

**The Flavor and Fragrance High Production Volume Consortia**  
**Robust Summaries for Terpenoid Primary Alcohols and Related Esters**

**FFHPVC Terpene Consortium Registration Number**

The evaluation of the quality of the following data uses a systematic approach described by Klimisch [Klimisch *et al.*, 1996]. Based on criteria relating to international testing standards for categorizing data reliability, four reliability categories have been established. The following categories are:

- Reliability code 1.      Reliable without restrictions
- Reliability code 2.      Reliable with restrictions
- Reliability code 3.      Not reliable
- Reliability code 4.      Not assignable

## **1 Chemical and Physical Properties**

### **1.1 Boiling Point**

<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9
<b>GLP</b>	NG
<b>Year</b>	1989
<b>Boiling Point</b>	225 °C
<b>Pressure</b>	1013 (760 mm Hg)
<b>Pressure Unit</b>	Millibars
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Basic data given and comparable to guidelines/standards.
<b>References</b>	Givaudan-Roure (1989) Determination of the ready biodegradability of d,l-citronellol. Unpublished report to Fragrance Materials Association.

<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1
<b>GLP</b>	NG

<b>Boiling Point</b>	230 °C
<b>Pressure</b>	760
<b>Pressure Unit</b>	mm Hg
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Basic data given and comparable to guidelines/standards.
<b>References</b>	Fragrance Materials Association (FMA) Reported values for boiling point.
<b>Substance Name</b>	Nerol
<b>CAS</b>	106-25-2
<b>GLP</b>	NG
<b>Boiling Point</b>	225 °C
<b>Pressure</b>	760
<b>Pressure Unit</b>	mm Hg
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Basic data given and comparable to guidelines/standards.
<b>References</b>	Fragrance Materials Association (FMA) Reported values for boiling point.
<b>Substance Name</b>	Citral
<b>CAS</b>	5392-40-5
<b>Remarks for Substance</b>	Substance supported under SIDS
<b>GLP</b>	NG
<b>Boiling Point</b>	230 °C
<b>Pressure</b>	760
<b>Pressure Unit</b>	mm Hg
<b>Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Basic data given and comparable to guidelines/standards.
<b>References</b>	Fragrance Materials Association (FMA) Reported values for boiling point.
<b>Substance Name</b>	Acetylated myrcene (data given for major component, geranyl acetate)
<b>CAS</b>	68412-04-4
<b>GLP</b>	NG
<b>Boiling Point</b>	244 °C

<b>Pressure</b>	760
<b>Pressure Unit</b>	mm Hg
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Basic data given and comparable to guidelines/standards.
<b>References</b>	Fragrance Materials Association (FMA) Reported values for boiling point.

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<b>Substance Name</b>	Acetylated myrcene (data given for major component, neryl acetate)
<b>CAS</b>	68412-04-4
<b>GLP</b>	NG
<b>Boiling Point</b>	231 °C
<b>Pressure</b>	760
<b>Pressure Unit</b>	mm Hg
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Basic data given and comparable to guidelines/standards.
<b>References</b>	Fragrance Materials Association (FMA) Reported values for boiling point.

## 1.2 Vapor Pressure

<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9
<b>Method/guideline</b>	Measured
<b>Year</b>	1995
<b>Vapor Pressure</b>	0.0095 kPa (0.071 mm Hg)
<b>Temperature</b>	30 °C
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions
<b>Remarks for Data Reliability</b>	Basic data given and comparable to guidelines/standards.
<b>References</b>	Vuilleumier C., Flament I. And Sauvegrain P. (1995) Headspace analysis study of evaporation rate of perfume ingredients applied onto skin. International Journal of Cosmetic Science 17, 61-76.

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<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1
<b>Method/guideline</b>	Calculated

<b>Vapor Pressure</b>	0.003 kPa (0.023 mm Hg)
<b>Temperature</b>	20 °C
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Basic data given and comparable to guidelines/standards.
<b>References</b>	Fragrance Materials Association (FMA). Reported values for vapor pressure.

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<b>Substance Name</b>	Nerol
<b>CAS</b>	106-25-2
<b>Method/guideline</b>	Calculated
<b>Vapor Pressure</b>	0.008 kPa (0.060 mm Hg)
<b>Temperature</b>	20 °C
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Basic data given and comparable to guidelines/standards.
<b>References</b>	Fragrance Materials Association (FMA). Reported values for vapor pressure.

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<b>Substance Name</b>	Citral
<b>CAS</b>	5392-40-5
<b>Remarks for substance.</b>	Substance supported under SIDS
<b>Method/guideline</b>	Calculated
<b>Vapor Pressure</b>	0.009 kPa (0.068 mm Hg)
<b>Temperature</b>	20 °C
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Basic data given and comparable to guidelines/standards.
<b>References</b>	Fragrance Materials Association (FMA). Reported values for vapor pressure.

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<b>Substance Name</b>	Acetylated myrcene (data for principal component geranyl acetate)
<b>CAS</b>	68412-04-4
<b>Remarks for substance.</b>	Substance supported under SIDS
<b>Method/guideline</b>	Calculated
<b>Vapor Pressure</b>	0.004 kPa (0.03 mm Hg)
<b>Temperature</b>	25 °C

<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Basic data given and comparable to guidelines/standards.
<b>References</b>	Fragrance Materials Association (FMA). Reported values for vapor pressure.

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<b>Substance Name</b>	Acetylated myrcene (data for principal component neryl acetate)
<b>CAS</b>	68412-04-4
<b>Remarks for substance.</b>	Substance supported under SIDS
<b>Method/guideline</b>	Calculated
<b>Vapor Pressure</b>	0.003 kPa (0.02 mm Hg)
<b>Temperature</b>	25 °C
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Basic data given and comparable to guidelines/standards.
<b>References</b>	Fragrance Materials Association (FMA). Reported values for vapor pressure.

### 1.3 Octanol/Water Partition Coefficient

<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9
<b>Method/guideline</b>	OECD Guideline No. 117; Reference substances = Thiourea, Acetophenone, Benzophenone, Naphthalene, 1,2,4-Trichlorobenzene
<b>GLP</b>	Yes
<b>Year</b>	1991
<b>Remarks for Test Conditions</b>	Reverse phase HPLC
<b>Log Pow</b>	3.1
<b>Remarks for Results</b>	Average retention time: 5.01
<b>Conclusion Remarks</b>	Good correlation with calculated log Pow of 3.56
<b>Data Qualities Reliabilities</b>	Reliability code 1. Reliable without restrictions.
<b>Remarks for Data Reliability</b>	Guideline study. The log Kow compares well with the calculated value. Data are considered reliable.
<b>References</b>	Givaudan-Roure (1991) Partition coefficient n-octanol/water of d,l-citronellol. Private communication to FMA.

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<b>Substance Name</b>	Geraniol
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<b>CAS</b>	106-24-1
<b>Method/guideline</b>	Calculated
<b>GLP</b>	NG
<b>Log Pow</b>	3.47
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Calculated Log Kow compares well with the measured value for the very closely related citronellol. Data are considered reliable.
<b>References</b>	Syracuse Research Corporation (SRC). Private communication to FMA.

<b>Substance Name</b>	Nerol
<b>CAS</b>	106-25-2
<b>Method/guideline</b>	Calculated
<b>Log Pow</b>	3.47
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Calculated Log Kow compares well with the measured value for the very closely related citronellol. Data are considered reliable.
<b>References</b>	Syracuse Research Corporation (SRC). Private communication to FMA.

<b>Substance Name</b>	Citral
<b>CAS</b>	5392-40-5
<b>Remarks for substance</b>	Substance supported under SIDS.
<b>Method/guideline</b>	Calculated
<b>Log Pow</b>	3.45
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Calculated Log Kow compares well with the measured value for the very closely related citronellol. Data are considered reliable.
<b>References</b>	Syracuse Research Corporation (SRC). Private communication to FMA.

<b>Substance Name</b>	Acetylated myrcene (data for principal component neryl acetate)
<b>CAS</b>	68412-04-4
<b>Method/guideline</b>	Calculated
<b>Log Pow</b>	4.48
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.

<b>Remarks for Data Reliability</b>	Calculated Log Kow compares well with the measured value for the very closely related citronellol. Data are considered reliable.
<b>References</b>	Syracuse Research Corporation (SRC). Private communication to FMA.

<b>Substance Name</b>	Acetylated myrcene (data for principal component geranyl acetate)
<b>CAS</b>	68412-04-4
<b>Method/guideline</b>	Calculated
<b>Log Pow</b>	4.48
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Calculated Log Kow compares well with the measured value for the very closely related citronellol. Data are considered reliable.
<b>References</b>	Syracuse Research Corporation (SRC). Private communication to FMA.

#### 1.4 Water Solubility

<b>Substance Name</b>	dl-Citronellol
<b>CAS No.</b>	106-22-9
<b>Method/guideline</b>	Calculated at log Kow=3.56 (ESPKOW)
<b>Value (mg/L) at temperature</b>	211 mg/L
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Comparable to guidelines/standards.
<b>References</b>	ESPOW

<b>Substance Name</b>	Geraniol
<b>CAS No.</b>	106-24-1
<b>Method/guideline</b>	Calculated at log Kow=3.47 (ESPKOW)
<b>Value (mg/L) at temperature</b>	256 mg/L
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Comparable to guidelines/standards.
<b>References</b>	ESPOW

<b>Substance Name</b>	Nerol
<b>CAS No.</b>	106-25-2
<b>Method/guideline</b>	Calculated at log Kow=3.47 (ESPKOW)
<b>Value (mg/L) at temperature</b>	256 mg/L
<b>Data Qualities Reliabilities Remarks for Data Reliability</b>	Reliability code 2. Reliable with restrictions. Comparable to guidelines/standards.
<b>References</b>	ESPOW

<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9
<b>GLP</b>	Not given
<b>Year</b>	1990
<b>Value (mg/L) at temperature</b>	0.03% w/V (300 mg/L)
<b>Data Qualities Reliabilities Remarks for Data Reliability</b>	Reliability code 2. Reliable with restrictions. Basic data given.
<b>References</b>	Bush Boake Allen, Inc (BBA) (1990) Biodegradability of geraniol and d,l-citronellol. Private communication to FMA.

<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1
<b>GLP</b>	Not given
<b>Year</b>	1990
<b>Value (mg/L) at temperature</b>	0.06% w/V (600 mg/L)
<b>Data Qualities Reliabilities Remarks for Data Reliability</b>	Reliability code 2. Reliable with restrictions. Basic data given.
<b>References</b>	Bush Boake Allen, Inc (BBA) (1990) Biodegradability of geraniol and d,l-citronellol Private Communication to FMA.

<b>Substance Name</b>	Acetylated myrcene (data for principal component geranyl acetate)
<b>CAS</b>	68412-04-4
<b>Method/guideline</b>	Calculated
<b>Value (mg/L) at temperature</b>	6.9 mg/L at 25 °C
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.

<b>Remarks for Data Reliability</b>	Comparable to guidelines/standards.
<b>References</b>	ESPOW

<b>Substance Name</b>	Acetylated myrcene (data for principal component neryl acetate)
<b>CAS</b>	68412-04-4
<b>Method/guideline</b>	Calculated
<b>Value (mg/L) at temperature</b>	6.9 mg/L at 25 °C
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Comparable to guidelines/standards.
<b>References</b>	ESPOW

## 2 Environmental Fate and Pathways

### 2.1 Photodegradation

<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9
<b>Method/guideline</b>	Calculation
<b>Test Type</b>	AOPWIN
<b>Half life t1/2</b>	1.3 hrs.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
<b>References</b>	AOPWIN

<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1
<b>Method/guideline</b>	Calculation
<b>Test Type</b>	AOPWIN
<b>Half life t1/2</b>	19 mins.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
<b>References</b>	AOPWIN

<b>Substance Name</b>	Nerol
<b>CAS</b>	106-25-2
<b>Method/guideline</b>	Calculation
<b>Test Type</b>	AOPWIN
<b>Half life t1/2</b>	19 mins.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable
<b>References</b>	AOPWIN

<b>Substance Name</b>	Citral (mixture of geranial and neral, 93:7)
<b>CAS</b>	5392-40-5
<b>Method/guideline</b>	Calculation
<b>Test Type</b>	AOPWIN

<b>Half-life t<sub>1/2</sub></b>	0.94 hrs.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
<b>References</b>	AOPWIN

<b>Substance Name</b>	Acetylated myrcene (data for principal component geranyl acetate)
<b>CAS</b>	68412-04-4
<b>Method/guideline</b>	Calculation
<b>Test Type</b>	AOPWIN
<b>Half life t<sub>1/2</sub></b>	19 mins.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
<b>References</b>	AOPWIN

<b>Substance Name</b>	Acetylated myrcene (data for principal component neryl acetate)
<b>CAS</b>	68412-04-4
<b>Method/guideline</b>	Calculation
<b>Test Type</b>	AOPWIN
<b>Half life t<sub>1/2</sub></b>	19 mins.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
<b>References</b>	AOPWIN

## 2.2 Stability in Water

<b>Substance Name</b>	Acetylated myrcene (acetylated myrcene is the process name for geranyl acetate. Data is for the dihydroisomer of geranyl acetate, citronellyl acetate)
<b>CAS No.</b>	68412-04-4
<b>Method/guideline</b>	Hydrolysis in simulated intestinal fluid (Longland, 1977)

<b>Test Type</b>	Ester hydrolysis in simulated intestinal fluid
<b>Year</b>	1977
<b>Duration (days)</b>	2 hours
<b>Analytical procedures</b>	Citronellyl acetate (15 uL/L) was incubated with pancreatin at a pH=7.5 in 0.5 M phosphate buffer at 37 C for 2 hours. The extent of hydrolysis was measured by gas-liquid chromatography.
<b>Temperature</b>	37 °C
<b>Nominal</b>	15 uL/L
<b>Degradation %</b>	100% hydrolysis
<b>Half-life t<sub>1/2</sub></b>	<1 hour
<b>Breakdown products</b>	Citronellol and acetic acid
<b>Conclusion remarks</b>	Citronellyl acetate was completely hydrolyzed in 2 hrs at pH7.5.
<b>Data Qualities Reliabilities</b>	Reliability code 1. Reliable without restrictions.
<b>Remarks for Data Reliability</b>	Data on citronellyl ester consistent with data for 24 other aliphatic and aromatic esters.
<b>References</b>	Grundschober F. (1977) Toxicological assessment of flavouring esters. Toxicology, 8:387-390.

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<b>Substance Name</b>	Acetylated myrcene (acetylated myrcene is the process name for geranyl acetate. Data is for the dihydroisomer of geranyl acetate, citronellyl phenylacetate)
<b>CAS No.</b>	68412-04-4
<b>Method/guideline</b>	Hydrolysis in simulated intestinal fluid (Longland, 1977)
<b>Test Type</b>	Ester hydrolysis in simulated intestinal fluid
<b>Year</b>	1977
<b>Duration (days)</b>	2 hours
<b>Analytical procedures</b>	Citronellyl phenylacetate (<18 uL/L) was incubated with pancreatin at a pH=7.5 in 0.5 M phosphate buffer at 37 C for 2 hours. The extent of hydrolysis was measured by gas-liquid chromatography.
<b>Temperature</b>	37 °C
<b>Nominal</b>	<18 uL/L
<b>Degradation %</b>	60% hydrolysis in 2 hrs.
<b>Half-life t<sub>1/2</sub></b>	<2 hours
<b>Breakdown products</b>	Citronellol and phenylacetic acid

<b>Conclusion remarks</b>	Citronellyl phenylacetate was completely hydrolyzed in 2 hours at pH 7.5.
<b>Data Qualities Reliabilities</b>	Reliability code 1. Reliable without restrictions.
<b>Remarks for Data Reliability</b>	Data on citronellyl ester consistent with data for 24 other aliphatic and aromatic esters.
<b>References</b>	Grundschober F. (1977) Toxicological assessment of flavouring esters. Toxicology 8:387-390.

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<b>Substance Name</b>	Acetylated myrcene (acetylated myrcene is the process name for a mixture containing mainly nerol and geranyl acetate. Data is for geranyl acetate)
<b>CAS No.</b>	68412-04-4
<b>Method/guideline</b>	Calculation
<b>Test Type</b>	Base/Acid-Catalyzed Hydrolysis
<b>Temperature</b>	25 °C
<b>Degradation %</b>	100% hydrolysis
<b>Half-life t<sub>1/2</sub></b>	23.14 days at pH=8: 231.4 days at pH=7
<b>Breakdown products</b>	Geraniol and acetic acid
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
<b>References</b>	AOPWIN

## 2.3 Biodegradation

<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9
<b>Remarks for Substance</b>	96.1% citronellol
<b>Method</b>	OECD 301 C
<b>Test Type</b>	Modified MITI
<b>GLP</b>	No
<b>Year</b>	1987
<b>Contact time (units)</b>	28 days
<b>Innoculum</b>	Activated sludge from 2 sewage treatment plants mixed with soil from bank of Rhone river.

<b>Remarks for Test Conditions</b>	108 mg/l at 20 °C for 28 days
<b>Degradation % after time</b>	65% at 28 days
<b>Time required for 10% degradation</b>	9 days
<b>10 day window criteria</b>	Yes
<b>Total degradation</b>	No
<b>Conclusion remarks</b>	Readily biodegradable
<b>Data Qualities Reliabilities</b>	Reliability code 1. Reliable without restrictions.
<b>Remarks for Data Reliability</b>	Guideline study.
<b>References</b>	Givaudan-Roure (1989) Determination of the ready biodegradability of d,l-citronellol. Unpublished report to FMA.

<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9
<b>Remarks for Substance</b>	96% mixture of <i>d,l</i> -citronellol
<b>Method</b>	Method F
<b>Test Type</b>	DOC - Method F from Blue book series, 1991
<b>GLP</b>	Yes
<b>Year</b>	1990
<b>Contact time (units)</b>	28 days
<b>Innoculum</b>	Activated sludge from local STP
<b>Remarks for Test Conditions</b>	41.6 mg DOC/l at 20 °C for 28 days
<b>Degradation % after time</b>	100% at 15 days
<b>Results</b>	100 % biodegradation after 15 days.
<b>Time required for 10% degradation</b>	< 1 day
<b>10 day window criteria</b>	Yes
<b>Total degradation</b>	Yes
<b>Conclusion remarks</b>	Readily biodegradable
<b>Data Qualities Reliabilities</b>	Reliability code 1. Reliable without restrictions.
<b>Remarks for Data Reliability</b>	Guideline study.
<b>References</b>	Bush Boake Allen, Inc (BBA) (1990) Biodegradability of geraniol and d,l-citronellol Private communication to FMA.

<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1

<b>Remarks for Substance</b>	Mixture of geraniol (50%), nerol (26%) and citronellol (18%)
<b>Method</b>	OECD 301B
<b>Test Type</b>	CO2 evolution
<b>GLP</b>	Yes
<b>Year</b>	1994
<b>Contact time (units)</b>	28 days
<b>Innoculum</b>	Secondary effluent from sludge from local STP
<b>Remarks for Test Conditions</b>	10 mg/l organic carbon at 20 °C for 28 days
<b>Degradation % after time</b>	100% at 28 days
<b>Time required for 10% degradation</b>	<7 days
<b>10 day window criteria</b>	Yes
<b>Total degradation</b>	Yes
<b>Conclusion remarks</b>	Readily biodegradable
<b>Data Qualities Reliabilities</b>	Reliability code 1. Reliable without restrictions.
<b>Remarks for Data Reliability</b>	Guideline study.
<b>References</b>	Quest International Ltd. (1994) The ultimate biodegradability of citronellol in the sealed vessel test. Private communication to FMA.

<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1
<b>Remarks for Substance</b>	99% mixture of geraniol (>70%) and nerol (<30%). EOA specification 16.
<b>Method</b>	Method F
<b>Test Type</b>	DOC - Method F from Blue book series, 1991
<b>GLP</b>	No
<b>Year</b>	1990
<b>Contact time (units)</b>	28 days
<b>Innoculum</b>	Activated sludge from local STP
<b>Remarks for Test Conditions</b>	42.0 mg DOC/l at 20 °C for 28 days
<b>Degradation % after time</b>	100% at 15 days
<b>Time required for 10% degradation</b>	< 1 day
<b>10 day window criteria</b>	Yes
<b>Total degradation</b>	Yes

<b>Conclusion remarks</b>	Readily biodegradable
<b>Data Qualities Reliabilities</b>	Reliability code 1. Reliable without restrictions.
<b>Remarks for Data Reliability</b>	Guideline study.
<b>References</b>	Bush Boake Allen, Inc (BBA) (1990) Biodegradability of geraniol and d,l-citronellol. Private communication to FMA.

<b>Substance Name</b>	Citral
<b>CAS</b>	5392-40-5
<b>Remarks for Substance</b>	94% pure - 44% <i>cis</i> (neral) and 50% <i>trans</i> (geranial)
<b>Method</b>	OECD 301B
<b>Test Type</b>	CO2 evolution
<b>GLP</b>	No
<b>Year</b>	1994
<b>Contact time (units)</b>	28 days
<b>Innoculum</b>	Secondary effluent from sludge from local STP
<b>Remarks for Test Conditions</b>	10 mg/l organic carbon at 20 °C for 28 days
<b>Degradation % after time</b>	92.1% at 28 days
<b>Time required for 10% degradation</b>	< 4 days
<b>10 day window criteria</b>	Yes
<b>Total degradation</b>	Yes
<b>Classification</b>	Not given
<b>Breakdown products (transient or stable?)</b>	Not given
<b>Conclusion remarks</b>	Readily biodegradable
<b>Data Qualities Reliabilities</b>	Reliability code 1. Reliable without restrictions.
<b>Remarks for Data Reliability</b>	Guideline study.
<b>References</b>	Quest International Ltd. (1994) The ultimate biodegradability of citronellol in the sealed vessel test. Private communication to FMA.

<b>Substance Name</b>	Citral
<b>CAS</b>	5392-40-5
<b>Method</b>	Method F
<b>Test Type</b>	DOC - Method F from Blue book series, 1991
<b>GLP</b>	No

<b>Year</b>	1990
<b>Contact time (units)</b>	28 days
<b>Innoculum</b>	Activated sludge from local STP
<b>Remarks for Test Conditions</b>	40.3 mg DOC/l at 20 °C for 28 days
<b>Degradation % after time</b>	99.5% at 19 days
<b>Kinetic</b>	Not given
<b>Time required for 10% degradation</b>	< 1 day
<b>10 day window criteria</b>	Yes
<b>Total degradation</b>	Yes
<b>Classification</b>	Not given
<b>Breakdown products (transient or stable?)</b>	Not given
<b>Conclusion remarks</b>	Readily biodegradable
<b>Data Qualities Reliabilities</b>	Reliability code 1. Reliable without restrictions.
<b>Remarks for Data Reliability</b>	Guideline study
<b>References</b>	Bush Boake Allen, Inc (BBA) (1990) Biodegradability of geraniol and d,l-citronellol. Private communication to FMA.

<b>Substance Name</b>	Acetylated myrcene
<b>CAS</b>	68412-04-4
<b>Remarks for Substance</b>	Acetylated myrcene is a mixture that is primarily (62%) acetate esters of nerol and geraniol.
<b>Method</b>	OECD 301B
<b>Test Type</b>	CO2 evolution
<b>GLP</b>	Not given
<b>Year</b>	1991
<b>Contact time (units)</b>	28 days
<b>Innoculum</b>	Secondary effluent from sludge from local STP
<b>Remarks for Test Conditions</b>	10 mg/l organic carbon at 20 °C for 28 days
<b>Degradation % after time</b>	82.2% at 28 days
<b>Results</b>	The requirements for ready and ultimate biodegradability were met.
<b>Kinetic</b>	Not given
<b>Time required for 10% degradation</b>	< 4 days

<b>10 day window criteria</b>	Yes
<b>Total degradation</b>	Yes
<b>Classification</b>	Not given
<b>Breakdown products (transient or stable?)</b>	Not given
<b>Conclusion remarks</b>	Readily biodegradable
<b>Data Qualities Reliabilities</b>	Reliability code 1. Reliable without restrictions.
<b>Remarks for Data Reliability</b>	Guideline study.
<b>References</b>	Birch R. R. and Fletcher R. J. (1991) The application of dissolved inorganic carbon measurements to the study of aerobic biodegradability. Chemosphere 23(4), 507-524.

## 2.4 Fugacity

<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, log Kow, estimated MP, water solubility
<b>Year</b>	1999
<b>Media</b>	Soil
<b>Estimated Distribution and Media Concentration</b>	42.1%
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.
<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9
<b>Model Conditions</b>	20 °C

<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, log Kow, estimated MP, water solubility
<b>Year</b>	1999
<b>Media</b>	Air-Water Partition Coefficient
<b>Absorption coefficient</b>	0.001
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, log Kow, estimated MP, water solubility
<b>Year</b>	1999
<b>Media</b>	Fish
<b>Estimated Distribution and Media Concentration</b>	0.0024%
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.
<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9
<b>Model Conditions</b>	20 °C

<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, log Kow, estimated MP, water solubility
<b>Year</b>	1999
<b>Media</b>	Sediment
<b>Estimated Distribution and Media Concentration</b>	0.94%
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.
<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, log Kow, estimated MP, water solubility
<b>Year</b>	1999
<b>Media</b>	Aerosol
<b>Estimated Distribution and Media Concentration</b>	0.00024%
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.
<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9

<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, log Kow, estimated MP, water solubility
<b>Year</b>	1999
<b>Media</b>	Water
<b>Estimated Distribution and Media Concentration</b>	37.8%
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, log Kow, estimated MP, water solubility
<b>Year</b>	1999
<b>Media</b>	Air
<b>Estimated Distribution and Media Concentration</b>	19.2%
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.
<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9

<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, log Kow, estimated MP, water solubility
<b>Year</b>	1999
<b>Media</b>	Aerosol-Air Partition Coefficient
<b>Absorption coefficient</b>	632000
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>Reference</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, log Kow, estimated MP, water solubility
<b>Year</b>	1999
<b>Media</b>	Fish-Water Partition Coefficient
<b>Absorption coefficient</b>	62.9
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.
<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9
<b>Model Conditions</b>	20 °C

<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, log Kow, estimated MP, water solubility
<b>Year</b>	1999
<b>Media</b>	Suspended Sediment-Water Partition Coefficient
<b>Absorption coefficient</b>	155
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

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<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, log Kow, estimated MP, water solubility
<b>Year</b>	1999
<b>Media</b>	Sediment-Water Partition Coefficient
<b>Absorption coefficient</b>	49.6
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

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<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model

<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, log Kow, estimated MP, water solubility
<b>Year</b>	1999
<b>Media</b>	Soil-Water Partition Coefficient
<b>Absorption coefficient</b>	24.8
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

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<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, log Kow, estimated MP, water solubility
<b>Year</b>	1999
<b>Media</b>	Suspended Sediment
<b>Estimated Distribution and Media Concentration</b>	0.029%
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

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<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model

<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, water solubility, estimated log Kow & MP
<b>Year</b>	1999
<b>Media</b>	Air
<b>Estimated Distribution and Media Concentration</b>	7.93%
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

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<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, water solubility, estimated log Kow & MP,
<b>Year</b>	1999
<b>Media</b>	Suspended Sediment
<b>Estimated Distribution and Media Concentration</b>	0.045%
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

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<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1
<b>Model Conditions</b>	20 °C

<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, water solubility, estimated log Kow & MP,
<b>Year</b>	1999
<b>Media</b>	Sediment
<b>Estimated Distribution and Media Concentration</b>	1.46%
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.
<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, water solubility, estimated log Kow & MP
<b>Year</b>	1999
<b>Media</b>	Soil
<b>Estimated Distribution and Media Concentration</b>	65.50%
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.
<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1

<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, water solubility, estimated log Kow & MP
<b>Year</b>	1999
<b>Media</b>	Water
<b>Estimated Distribution and Media Concentration</b>	25.06%
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, water solubility, estimated log Kow & MP
<b>Year</b>	1999
<b>Media</b>	Aerosol-Air Partition Coefficient
<b>Absorption coefficient</b>	2000000
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.
<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1

<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, water solubility, estimated log Kow & MP
<b>Year</b>	1999
<b>Media</b>	Fish-Water Partition Coefficient
<b>Absorption coefficient</b>	148
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, water solubility, estimated log Kow & MP
<b>Year</b>	1999
<b>Media</b>	Suspended Sediment-Water Partition Coefficient
<b>Absorption coefficient</b>	363
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.
<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1
<b>Model Conditions</b>	20 °C

<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, water solubility, estimated log Kow & MP
<b>Year</b>	1999
<b>Media</b>	Sediment-Water Partition Coefficient
<b>Absorption coefficient</b>	116.2
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, water solubility, estimated log Kow & MP
<b>Year</b>	1999
<b>Media</b>	Fish
<b>Estimated Distribution and Media Concentration</b>	0.0037%
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1
<b>Model Conditions</b>	20 °C

<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, water solubility, estimated log Kow & MP
<b>Year</b>	1999
<b>Media</b>	Air-Water Partition Coefficient
<b>Absorption coefficient</b>	0.00063
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, water solubility, estimated log Kow & MP
<b>Year</b>	1999
<b>Media</b>	Aerosol
<b>Estimated Distribution and Media Concentration</b>	0.00032%
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1
<b>Model Conditions</b>	20 °C

<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, water solubility, estimated log Kow & MP
<b>Year</b>	1999
<b>Media</b>	Soil-Water Partition Coefficient
<b>Absorption coefficient</b>	58.1
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

<b>Substance Name</b>	Nerol
<b>CAS</b>	106-25-2
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, water solubility, estimated log Kow & MP
<b>Year</b>	1999
<b>Media</b>	Soil
<b>Estimated Distribution and Media Concentration</b>	65.50%
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restrictions because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

<b>Substance Name</b>	Nerol
<b>CAS</b>	106-25-2
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model

<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, water solubility, estimated log Kow & MP
<b>Year</b>	1999
<b>Media</b>	Air-Water Partition Coefficient
<b>Absorption coefficient</b>	0.00063
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

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<b>Substance Name</b>	Nerol
<b>CAS</b>	106-25-2
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, water solubility, estimated log Kow & MP
<b>Year</b>	1999
<b>Media</b>	Fish
<b>Estimated Distribution and Media Concentration</b>	0.0037%
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

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<b>Substance Name</b>	Nerol
<b>CAS</b>	106-25-2
<b>Model Conditions</b>	20 C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model

<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, water solubility, estimated log Kow & MP
<b>Year</b>	1999
<b>Media</b>	Sediment
<b>Estimated Distribution and Media Concentration</b>	1.46%
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.
<b>Substance Name</b>	Nerol
<b>CAS</b>	106-25-2
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, water solubility, estimated log Kow & MP
<b>Year</b>	1999
<b>Media</b>	Aerosol
<b>Estimated Distribution and Media Concentration</b>	0.00032%
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.
<b>Substance Name</b>	Nerol
<b>CAS</b>	106-25-2
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model

<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, water solubility, estimated log Kow & MP
<b>Year</b>	1999
<b>Media</b>	Water
<b>Estimated Distribution and Media Concentration</b>	25.06%
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>Reference</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

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<b>Substance Name</b>	Nerol
<b>CAS</b>	106-25-2
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, water solubility, estimated log Kow & MP
<b>Year</b>	1999
<b>Media</b>	Air
<b>Estimated Distribution and Media Concentration</b>	7.93%
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

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<b>Substance Name</b>	Nerol
<b>CAS</b>	106-25-2
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model

<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, water solubility, estimated log Kow & MP
<b>Year</b>	1999
<b>Media</b>	Aerosol-Air Partition Coefficient
<b>Absorption coefficient</b>	2000000
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

<b>Substance Name</b>	Nerol
<b>CAS</b>	106-25-2
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, water solubility, estimated log Kow & MP
<b>Year</b>	1999
<b>Media</b>	Fish-Water Partition Coefficient
<b>Absorption coefficient</b>	148
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

<b>Substance Name</b>	Nerol
<b>CAS</b>	106-25-2
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model

<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, water solubility, estimated log Kow & MP
<b>Year</b>	1999
<b>Media</b>	Suspended Sediment-Water Partition Coefficient
<b>Absorption coefficient</b>	363
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

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<b>Substance Name</b>	Nerol
<b>CAS</b>	106-25-2
<b>Remarks for Substance</b>	
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, water solubility, estimated log Kow & MP
<b>Year</b>	1999
<b>Media</b>	Sediment-Water Partition Coefficient
<b>Absorption coefficient</b>	116.2
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

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<b>Substance Name</b>	Nerol
<b>CAS</b>	106-25-2
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model

<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, water solubility, estimated log Kow & MP
<b>Year</b>	1999
<b>Remarks for Test Conditions</b>	
<b>Media</b>	Soil-Water Partition Coefficient
<b>Absorption coefficient</b>	58.1
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

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<b>Substance Name</b>	Nerol
<b>CAS</b>	106-25-2
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	MW, VP, water solubility, estimated log Kow & MP
<b>Year</b>	1999
<b>Media</b>	Suspended Sediment
<b>Estimated Distribution and Media Concentration</b>	0.045%
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

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<b>Substance Name</b>	Acetylated myrcene
<b>CAS</b>	68412-04-4
<b>Remarks for Substance</b>	All data estimated based on the properties of the principal components

<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	Estimated MW, VP, log Kow, MP & water solubility
<b>Year</b>	1999
<b>Media</b>	Air
<b>Estimated Distribution and Media Concentration</b>	57.6%
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

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<b>Substance Name</b>	Acetylated myrcene
<b>CAS</b>	68412-04-4
<b>Remarks for Substance</b>	All data estimated based on the properties of the principal components
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	Estimated MW, VP, log Kow, MP & water solubility
<b>Year</b>	1999
<b>Media</b>	Fish
<b>Estimated Distribution and Media Concentration</b>	0.0023%
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

<b>Substance Name</b>	Acetylated myrcene
<b>CAS</b>	68412-04-4
<b>Remarks for Substance</b>	All data estimated based on the properties of the principal components
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	Estimated MW, VP, log Kow, MP & water solubility
<b>Year</b>	1999
<b>Media</b>	Suspended Sediment
<b>Estimated Distribution and Media Concentration</b>	0.028%
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

<b>Substance Name</b>	Acetylated myrcene
<b>CAS</b>	68412-04-4
<b>Remarks for Substance</b>	All data estimated based on the properties of the principal components
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used (title, version, ate)</b>	EQC V 2.11 Level I
<b>Input parameters</b>	Estimated MW, VP, log Kow, MP & water solubility
<b>Year</b>	1999
<b>Remarks for Test Conditions</b>	
<b>Media</b>	Sediment
<b>Estimated Distribution and Media Concentration</b>	0.89%

<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

<b>Substance Name</b>	Acetylated myrcene
<b>CAS</b>	68412-04-4
<b>Remarks for Substance</b>	All data estimated based on the properties of the principal components
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	Estimated MW, VP, log Kow, MP & water solubility
<b>Year</b>	1999
<b>Media</b>	Soil
<b>Estimated Distribution and Media Concentration</b>	40.1%
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered Reliability code 2. Reliable with restrictions. because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

<b>Substance Name</b>	Acetylated myrcene
<b>CAS</b>	68412-04-4
<b>Remarks for Substance</b>	All data estimated based on the properties of the principal components
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	Estimated MW, VP, log Kow, MP & water solubility

<b>Year</b>	1999
<b>Media</b>	Water
<b>Estimated Distribution and Media Concentration</b>	1.43%
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

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<b>Substance Name</b>	Acetylated myrcene
<b>CAS</b>	68412-04-4
<b>Remarks for Substance</b>	All data estimated based on the properties of the principal components
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	Estimated MW, VP, log Kow, MP & water solubility
<b>Year</b>	1999
<b>Media</b>	Aerosol-Air Partition Coefficient
<b>Absorption coefficient</b>	1200000
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

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<b>Substance Name</b>	Acetylated myrcene
<b>CAS</b>	6412-04-4
<b>Remarks for Substance</b>	All data estimated based on the properties of the principal components
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model

<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	Estimated MW, VP, log Kow, MP & water solubility
<b>Year</b>	1999
<b>Remarks for Test Conditions</b>	
<b>Media</b>	Fish-Water Partition Coefficient
<b>Absorption coefficient</b>	1580
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

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<b>Substance Name</b>	Acetylated myrcene
<b>CAS</b>	68412-04-4
<b>Remarks for Substance</b>	All data estimated based on the properties of the principal components
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	Estimated MW, VP, log Kow, MP & water solubility
<b>Year</b>	1999
<b>Media</b>	Suspended Sediment-Water Partition Coefficient
<b>Absorption coefficient</b>	3890
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

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<b>Substance Name</b>	Acetylated myrcene
<b>CAS</b>	68412-04-4

<b>Remarks for Substance</b>	All data estimated based on the properties of the principal components
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	Estimated MW, VP, log Kow, MP & water solubility
<b>Year</b>	1999
<b>Media</b>	Sediment-Water Partition Coefficient
<b>Absorption coefficient</b>	1240
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

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<b>Substance Name</b>	Acetylated myrcene
<b>CAS</b>	68412-04-4
<b>Remarks for Substance</b>	All data estimated based on the properties of the principal components
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	Estimated MW, VP, log Kow, MP & water solubility
<b>Year</b>	1999
<b>Media</b>	Air-Water Partition Coefficient
<b>Absorption coefficient</b>	0.080
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

<b>Substance Name</b>	Acetylated myrcene
<b>CAS</b>	68412-04-4
<b>Remarks for Substance</b>	All data estimated based on the properties of the principal components
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	Estimated MW, VP, log Kow, MP & water solubility
<b>Year</b>	1999
<b>Media</b>	Aerosol
<b>Estimated Distribution and Media Concentration</b>	0.0014%
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.

<b>Substance Name</b>	Acetylated myrcene
<b>CAS</b>	68412-04-4
<b>Remarks for Substance</b>	All data estimated based on the properties of the principal components
<b>Model Conditions</b>	20 °C
<b>Test Type</b>	Environmental Equilibrium Partitioning Model
<b>Method</b>	Mackay
<b>Model Used</b>	EQC V 2.11 Level I
<b>Input parameters</b>	Estimated MW, VP, log Kow, MP & water solubility
<b>Year</b>	1999
<b>Media</b>	Soil-Water Partition Coefficient
<b>Absorption coefficient</b>	622
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism.
<b>References</b>	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.



### 3 Ecotoxicity

#### 3.1 Acute Toxicity to Fish

<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9
<b>Method/guideline</b>	ECOSAR
<b>Test Type</b>	Calculated based on measured Kow
<b>Species/Strain/Supplier</b>	Fish
<b>Exposure period (unit)</b>	96 hr
<b>Conclusion remarks</b>	LC50 = 10.7 mg/l
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
<b>References</b>	ECOSAR

<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1
<b>Method/guideline</b>	ECOSAR
<b>Test Type</b>	Calculated
<b>Species/Strain/Supplier</b>	Fish
<b>Exposure period (unit)</b>	96 hr
<b>Conclusion remarks</b>	LC50 = 0.57 mg/l (see Remarks for Reliability)
<b>Remarks for Data Reliability</b>	The data were obtained by a recognized SAR calculation method but are not consistent with chemical structure. Data are considered overly conservative by submitters.
<b>References</b>	ECOSAR

<b>Substance Name</b>	Nerol
<b>CAS</b>	106-25-2
<b>Method/guideline</b>	ECOSAR
<b>Test Type</b>	Calculated
<b>Species/Strain/Supplier</b>	Fish
<b>Exposure period (unit)</b>	96 hr
<b>Conclusion remarks</b>	LC50 = 0.57 mg/l (see Remarks for Reliability)
<b>Remarks for Data Reliability</b>	The data were obtained by a recognized SAR calculation method but are not consistent with chemical structure. Data are considered overly conservative by the submitters.

are considered overly conservative by the submitters.

<b>References</b>	ECOSAR
<b>Substance Name</b>	Citral
<b>CAS</b>	5392-40-5
<b>Method/guideline</b>	ECOSAR
<b>Test Type</b>	Calculated
<b>Species/Strain/Supplier</b>	Fish
<b>Exposure period (unit)</b>	96 hr
<b>Conclusion remarks</b>	LC50 = 4.5 mg/l
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized SAR calculation method but are not consistent with chemical structure. Data are considered overly conservative by the submitters.
<b>References</b>	ECOSAR
<b>Substance Name</b>	Acetylated myrcene (data given for major component, geranyl acetate)
<b>CAS</b>	68412-04-4
<b>Method/guideline</b>	ECOSAR
<b>Test Type</b>	Calculated
<b>Species/Strain/Supplier</b>	Fish
<b>Exposure period (unit)</b>	96 hr
<b>Conclusion remarks</b>	LC50 = 1.4 mg/l
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized SAR calculation method but are not consistent with chemical structure. Data are considered overly conservative by the submitters.
<b>References</b>	ECOSAR
<b>Substance Name</b>	Acetylated myrcene (data given for major component, neryl acetate)
<b>CAS</b>	68412-04-4
<b>Method/guideline</b>	ECOSAR
<b>Test Type</b>	Calculated
<b>Species/Strain/Supplier</b>	Fish
<b>Exposure period (unit)</b>	96 hr
<b>Conclusion remarks</b>	LC50 = 1.4 mg/l
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized SAR calculation method but are not consistent with chemical structure. Data are

but are not consistent with chemical structure. Data are considered overly conservative by the submitters.

## References

ECOSAR

### 3.2 Acute Toxicity to Aquatic Invertebrates

<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9
<b>Method/guideline</b>	ECOSAR
<b>Test Type</b>	Calculated based on measured Kow
<b>Analytical procedures</b>	Daphnia
<b>Test details</b>	48 hrs
<b>EC50, EL50, LC50, at 24,48 hours</b>	LC50=12.4 mg/l
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
<b>References</b>	ECOSAR

<b>Substance Name</b>	Citral
<b>CAS</b>	5392-40-5
<b>Remarks for Substance</b>	Substance supported under SIDS.
<b>Method/guideline</b>	ECOSAR
<b>Test Type</b>	Calculated
<b>Analytical procedures</b>	Daphnia
<b>Test details</b>	48 hrs
<b>EC50, EL50, LC0, at 24,48 hours</b>	LC50=1.1 mg/l
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
<b>References</b>	ECOSAR

<b>Substance Name</b>	Acetylated myrcene (data given for major component, neryl acetate)
<b>CAS</b>	68412-04-4
<b>Method/guideline</b>	ECOSAR
<b>Test Type</b>	Calculated

<b>Analytical procedures</b>	Daphnia
<b>Test details</b>	48 hrs
<b>EC50, EL50, LC0, at 24,48 hours</b>	LC50=0.86 mg/l
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
<b>References</b>	ECOSAR

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<b>Substance Name</b>	Acetylated myrcene (data given for major component, geranyl acetate)
<b>CAS</b>	68412-04-4
<b>Method/guideline</b>	ECOSAR
<b>Test Type</b>	Calculated
<b>Analytical procedures</b>	Daphnia
<b>Test details</b>	48 hrs
<b>EC50, EL50, LC0, at 24,48 hours</b>	LC50=0.86 mg/l
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
<b>References</b>	ECOSAR

### 3.3 Acute Toxicity To Aquatic Plants

<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9
<b>Method/guideline</b>	Plate Inhibition Assay [Ikawa, 1992]
<b>Test Type</b>	Algal Growth Inhibition Test
<b>Species/Strain/Supplier</b>	Green algae
<b>Exposure period (duration)</b>	48 hr
<b>Analytical Monitoring</b>	Net diameter of inhibition zone= total diameter-disk diameter (5mm)
<b>Remarks for Test Conditions</b>	Three disks containing the test solution were placed on a agar plate containing Chlorella p. and then exposed to fluorescent lights for 48 hours. Zone of inhibition measured on two separate occasions.
<b>Nominal Concentration as mg/L:</b>	100, 1000, or 10,000 mg/L

<b>Unit</b>	mg/L
<b>NOEC, LOEC</b>	NOEC=100 or 1000 mg/L, LOEC=10,000 mg/L
<b>Biological Observations</b>	Complete wipe out of yellow green algal lawn at 10,000 mg/L
<b>Statistical Evaluations?</b>	None
<b>Control Response Satisfactory</b>	Yes
<b>Conclusion remarks</b>	No effects on growth of <i>Chlorella p.</i> at 1000 mg/L. Authors noted that inhibition was also observed when solution disks at concentrations of 10,000 mg/L were separated from agar medium by Teflon disks.
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Data was reported in a peer-reviewed journal- <i>Journal of Chemical Ecology</i>
<b>References</b>	Ikawa M., Mosley S., and Barbero L. (1992) Inhibitory effects of terpene alcohols and aldehydes on growth of green alga <i>Chlorella pyrenoidosa</i> . <i>Journal of Chemical Ecology</i> <b>18</b> (10),1755-1760.

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<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1
<b>Method/guideline</b>	Plate Inhibition Assay [Ikawa, 1992]
<b>Test Type</b>	Algal Growth Inhibition Test
<b>Species/Strain/Supplier</b>	Green algae
<b>Exposure period (duration)</b>	48 hr
<b>Analytical Monitoring</b>	Net diameter of inhibition zone= total diameter-disk diameter (5mm)
<b>Remarks for Test Conditions</b>	Three disks containing the test solution were placed on an agar plate containing <i>Chlorella p.</i> and then exposed to fluorescent lights for 48 hours. Zone of inhibition measured on two separate occasions.
<b>Nominal Concentration as mg/L:</b>	100, 1000, or 10,000 mg/L
<b>Unit</b>	mg/L
<b>NOEC, LOEC</b>	NOEC=100 mg/L, LOEC=1000 mg/L
<b>Biological Observations</b>	Lightening of lawn color at 1000 mg/L. Complete wipe out of yellow green algal lawn at 10,000 mg/L
<b>Statistical Evaluations?</b>	None
<b>Control Response Satisfactory</b>	Yes

<b>Conclusion remarks</b>	No effects on growth of <i>Chlorella p.</i> at 100 mg/L. Authors noted that inhibition was also observed when solution disks at concentrations of 1000 or 10,000 mg/L were separated from agar medium by Teflon disks.
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Data was reported in a peer-reviewed journal- <i>Journal of Chemical Ecology</i>
<b>References</b>	Ikawa M., Mosley S., and Barbero L. (1992) Inhibitory effects of terpene alcohols and aldehydes on growth of green alga <i>Chlorella pyrenoidosa</i> . <i>Journal of Chemical Ecology</i> <b>18</b> (10),1755-1760.
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<b>Substance Name</b>	Nerol
<b>CAS</b>	106-25-2
<b>Method/guideline</b>	Plate Inhibition Assay [Ikawa, 1992]
<b>Test Type</b>	Algal Growth Inhibition Test
<b>Species/Strain/Supplier</b>	Green algae
<b>Exposure period (duration)</b>	48 hr
<b>Analytical Monitoring</b>	Net diameter of inhibition zone= total diameter-disk diameter (5mm)
<b>Remarks for Test Conditions</b>	Three disks containing the test solution were placed on a agar plate containing <i>Chlorella p.</i> and then exposed to fluorescent lights for 48 hours. Zone of inhibition measured on two separate occasions.
<b>Nominal Concentration as mg/L:</b>	100, 1000, or 10,000 mg/L
<b>Unit</b>	mg/L
<b>NOEC, LOEC</b>	NOEC=100 mg/L, LOEC=1000 mg/L
<b>Biological Observations</b>	Lightening of lawn color at 1000 mg/L. Complete wipe out of yellow green algal lawn at 10,000 mg/L
<b>Statistical Evaluations?</b>	None
<b>Control Response Satisfactory</b>	Yes
<b>Conclusion remarks</b>	No effects on growth of <i>Chlorella p.</i> at 100 mg/L. Authors noted that inhibition was also observed when solution disks at concentrations of 1000 or 10,000 mg/L were separated from agar medium by Teflon disks.
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Data was reported in a peer-reviewed journal- <i>Journal of Chemical Ecology</i>

**References**

Ikawa M., Mosley S., and Barbero L. (1992) Inhibitory effects of terpene alcohols and aldehydes on growth of green alga *Chlorella pyrenoidosa*. *Journal of Chemical Ecology* **18**(10),1755-1760.

<b>Substance Name</b>	Citral
<b>CAS</b>	5392-40-5
<b>Method/guideline</b>	Plate Inhibition Assay [Ikawa, 1992]
<b>Test Type</b>	Algal Growth Inhibition Test
<b>Species/Strain/Supplier</b>	Green algae
<b>Exposure period (duration)</b>	48 hr
<b>Analytical Monitoring</b>	Net diameter of inhibition zone= total diameter-disk diameter (5mm)
<b>Remarks for Test Conditions</b>	Three disks containing the test solution were placed on a agar plate containing <i>Chlorella p.</i> and then exposed to fluorescent lights for 48 hours. Zone of inhibition measured on two separate occasions.
<b>Nominal Concentration as mg/L:</b>	100, 1000, or 10,000 mg/L
<b>Unit</b>	mg/L
<b>NOEC, LOEC</b>	NOEC=100 mg/L, LOEC=1000 mg/L
<b>Biological Observations</b>	Complete wipe out of yellow green algal lawn at 1000 and 10,000 mg/L
<b>Statistical Evaluations?</b>	None
<b>Control Response Satisfactory</b>	Yes
<b>Conclusion remarks</b>	No effects on growth of <i>Chlorella p.</i> at 100 mg/L. Authors noted that inhibition was also observed when solution disks at concentrations of 1000 or 10,000 mg/L were separated from agar medium by Teflon disks.
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Data was reported in a peer-reviewed journal.
<b>References</b>	Ikawa M., Mosley S., and Barbero L. (1992) Inhibitory effects of terpene alcohols and aldehydes on growth of green alga <i>Chlorella pyrenoidosa</i> . <i>J. of Chem. Ecology</i> <b>18</b> (10),1755-1760.
<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9
<b>Method/guideline</b>	Calculated

<b>Test Type</b>	ECOSAR
<b>Species/Strain/Supplier</b>	Green algae
<b>Exposure period (duration)</b>	96 hr
<b>Conclusion remarks</b>	EC50 = 8.2 mg/l
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
<b>References</b>	ECOSAR

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<b>Substance Name</b>	Citral
<b>CAS</b>	5392-40-5
<b>Remarks for Substance</b>	Substance supported under SIDS.
<b>Method/guideline</b>	Calculated
<b>Test Type</b>	ECOSAR
<b>Species/Strain/Supplier</b>	Green algae
<b>Exposure period (duration)</b>	96 hr
<b>Conclusion remarks</b>	EC50 = 3.9 mg/l
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
<b>References</b>	ECOSAR

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<b>Substance Name</b>	Acetylated myrcene (data given for major component, neryl acetate)
<b>CAS</b>	68412-04-4
<b>Method/guideline</b>	Calculated
<b>Test Type</b>	ECOSAR
<b>Species/Strain/Supplier</b>	Green algae
<b>Exposure period (duration)</b>	96 hr
<b>Conclusion remarks</b>	EC50 = 0.12 mg/l
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
<b>References</b>	ECOSAR

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<b>Substance Name</b>	Acetylated myrcene (data given for major component, geranyl acetate)
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<b>CAS</b>	68412-04-4
<b>Method/guideline</b>	Calculated
<b>Test Type</b>	ECOSAR
<b>Species/Strain/Supplier</b>	Green algae
<b>Exposure period (duration)</b>	96 hr
<b>Conclusion remarks</b>	EC50 = 0.12 mg/l
<b>Remarks for Data Reliability</b>	The data are obtained by a recognized SAR calculation method and are consistent with chemical structure. Data are considered reliable.
<b>References</b>	ECOSAR

## 4 Human Health Data

### 4.1 Acute Toxicity

<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9
<b>Remarks for Substance</b>	Purity undetermined.
<b>Method/guideline</b>	NG
<b>Test Type</b>	Acute ED25
<b>GLP</b>	Not reported
<b>Year</b>	1977
<b>Species/Strain</b>	Mouse/CD-1
<b>Sex</b>	Female
<b># of animals per sex per dose</b>	5
<b>Vehicle</b>	None
<b>Route of administration</b>	Inhalation
<b>Remarks for test conditions</b>	The respiratory irritation potential of fragrance raw materials was assessed in CD-1 females by recording respiratory rate using a whole body plethysmograph. Mice, weighing between 23-28 grams were exposed to test materials for 1 minute using a nebulizer for aerosolization in a 2600 ml chamber. Materials shown to be sensory irritants were further tested in mice cannulated via the trachea & compared to an intact mouse breathing through its nose. Comparisons made were between the pre-exposure & exposure rate values for each material at each dose level. Materials were of undetermined purity.
<b>Value LD50 or LC50 with confidence limits</b>	ED25=990 micrograms/L
<b>Remarks for results</b>	Slight respiratory depression. Lower tract exposures not performed
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Basic data given and comparable to guidelines/standards.
<b>References</b>	Troy, W.R. (1977) Doctoral Dissertation: The comparative respiratory irritation potential of fourteen fragrance raw materials. Unpublished report to RIFM.
<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9
<b>Remarks for Substance</b>	Not reported

<b>Method/guideline</b>	NG
<b>Test Type</b>	Acute dermal LD50
<b>GLP</b>	Not reported
<b>Year</b>	1973
<b>Species/Strain</b>	Rabbits/New Zealand White
<b>Sex</b>	Not reported
<b># of animals per sex per dose</b>	5
<b>Vehicle</b>	None
<b>Route of administration</b>	Dermal
<b>Remarks for test conditions</b>	Five rabbits per dose were administered 0, 1.25, 2.5 or 5.0 g/kg bw citronellol. Animals were observed for toxic signs and death.
<b>Value LD50 or LC50 with confidence limits</b>	2.65 g/kg (95% C.L. 1.78-3.52 g/kg)
<b>Number of deaths at each dose level</b>	1.25 g/kg 0/5 deaths; 2.5 g/kg 2/5 deaths; 5 g/kg 5/5 deaths
<b>Remarks for results</b>	The LD50 was calculated to be 2.65 g/kg calculated LD50, 95% limits=1.78-3.52 gm/kg. Toxic signs were ataxia and papillary dilation.
<b>Conclusion remarks</b>	The LD50 was reported to be 2.65 g/kg bw (2650 mg/kg bw)
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Basic data given and comparable to guidelines/standards.
<b>References</b>	Moreno O. M. (1973) Acute oral toxicity studies on rats and rabbits. Unpublished report to RIFM.

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<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9
<b>Remarks for Substance</b>	Not reported
<b>Method/guideline</b>	NG
<b>Test Type</b>	Oral LD50
<b>GLP</b>	Not reported
<b>Year</b>	1973
<b>Species/Strain</b>	Rat
<b>Sex</b>	Not reported
<b># of animals per sex per dose</b>	10
<b>Vehicle</b>	None reported

<b>Route of administration</b>	Oral
<b>Remarks for test conditions</b>	Ten rats per dose level were administered 2050, 2560, 3200, 4000, or 5000 mg/kg bw citronellol and observed for fourteen days.
<b>Value LD50 or LC50 with confidence limits</b>	3450 mg/kg bw (95% C.L. 3210-3690 mg/kg bw)
<b>Number of deaths at each dose level</b>	2050 mg/kg 1/10 deaths; 2560 mg/kg 0/10 deaths; 3200 mg/kg 7/10 deaths; 4000 mg/kg 6/10 deaths; 5000 mg/kg 8/10 deaths
<b>Remarks for results</b>	Spontaneous activity reduced 20 min after administration. 2000 mg/kg bw spontaneous activity reduced. All animals affected 10-30 min after administration, peaked at 4-6 hr & returned to normal at 48 hr.
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Basic data given and comparable to guidelines/standards.
<b>References</b>	Moreno O. M. (1973) Acute oral toxicity studies on rats and rabbits. Unpublished report to RIFM.

<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1
<b>Remarks for Substance</b>	Purity undetermined
<b>Method/guideline</b>	Not given
<b>Test Type</b>	Acute ED25
<b>GLP</b>	Not reported
<b>Year</b>	1977
<b>Species/Strain</b>	Mouse/CD-1
<b>Sex</b>	Female
<b># of animals per sex per dose</b>	5
<b>Vehicle</b>	None
<b>Route of administration</b>	Inhalation
<b>Remarks for test conditions</b>	The respiratory irritation potential of fragrance raw materials was assessed in CD-1 females by recording respiratory rate using a whole body plethysmograph. Mice were exposed to test materials for 1 min using a nebulizer for aerosolization in a 2600 ml chamber. Materials shown to be sensory irritants were further tested in mice cannulated via the trachea & compared to an intact mouse breathing through its nose. Comparisons made were between the pre-exposure & exposure rate values for each material at each dose level. Materials were of undetermined purity.
<b>Value LD50 or LC50 with confidence limits</b>	ED25=570 micrograms/L

**confidence limits**

**Remarks for results** Mild moderate respiratory depression. No effects when inhaled through tracheal cannula.

**Data Qualities Reliabilities** Reliability code 2. Reliable with restrictions.

**Remarks for Data Reliability** Basic data given and comparable to guidelines/standards.

**References** Troy W.R. (1977) Doctoral Dissertation: The comparative respiratory irritation potential of fourteen fragrance raw materials. Unpublished report to RIFM.

<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1
<b>Remarks for Substance</b>	Not reported
<b>Method/guideline</b>	Litchfield-Wilcoxon, 1949 (FDA study)
<b>Test Type</b>	Oral LD50
<b>GLP</b>	Not reported
<b>Year</b>	1964
<b>Species/Strain</b>	Rat/Osborne-Mendel
<b>Sex</b>	Male and Female
<b># of animals per sex per dose</b>	5
<b>Vehicle</b>	None
<b>Route of administration</b>	Intubation
<b>Remarks for test conditions</b>	5 male and 5 female young adult Osborne-Mendel rats were fasted for 18 hrs prior to treatment. Animals were observed for toxic signs and death. The observation period was 2 wks.
<b>Value LD50 or LC50 with confidence limits</b>	3600 mg/kg bw (95% C.L. 2840-4570)
<b>Number of deaths at each dose level</b>	Not reported
<b>Remarks for results</b>	Slope function: 1.7 (95% C.L. 1.3-2.2). Toxic signs were depression, coma, and wet fur. Times of deaths were between 4-18 hours.
<b>Data Qualities Reliabilities</b>	Reliability code 1. Reliable without restrictions.
<b>Remarks for Data Reliability</b>	Guideline study
<b>References</b>	Jenner P.M., Hagan E.C., Taylor J.M., Cook E.L., Fitzhugh O.G. (1964) Food flavorings and compounds of related structure I. Acute Oral Toxicity. Fd. Cosmet. Toxicol. 2, 327-343.
<b>Substance Name</b>	Geraniol

<b>CAS</b>	106-24-1
<b>Remarks for Substance</b>	Not reported
<b>Method/guideline</b>	Litchfield and Wilcoxon, 1949
<b>Test Type</b>	Oral LD50
<b>GLP</b>	Not reported
<b>Year</b>	1962
<b>Species/Strain</b>	Mixed strains rat
<b>Sex</b>	Not reported
<b>Vehicle</b>	Propylene glycol
<b>Route of administration</b>	Gavage
<b>Remarks for test conditions</b>	Groups of 8 mixed breed rats weighing approximately 150 g were given geraniol at the following doses, 1, 5, 10, 100, 1000, 2000, 5000 mg/kg bw in propylene glycol by stomach tube & observed for 48 hr. A vehicle control was also administered.
<b>Value LD50 or LC50 with confidence limits</b>	4800 mg/kg bw (95% C.I. 2900-5900 mg/kg bw)
<b>Number of deaths at each dose level</b>	5000 mg/kg bw 3/5 deaths
<b>Remarks for results</b>	The LD50 reported was 4800 mg/kg bw.
<b>Conclusion remarks</b>	The LD50 reported was 4800 mg/kg bw.
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Basic data given and comparable to guidelines/standards.
<b>References</b>	Yamawaki T. (1962). Pharmacological effects of geraniol. Nippon Yakurigaku Zasshi, 58, 394-400.

  

<b>Substance Name</b>	Nerol
<b>CAS</b>	106-25-2
<b>Remarks for Substance</b>	Purity undetermined.
<b>Method/guideline</b>	NG
<b>Test Type</b>	Acute ED25
<b>GLP</b>	Not reported
<b>Year</b>	1977
<b>Species/Strain</b>	Mouse/CD-1
<b>Sex</b>	Female
<b># of animals per sex per dose</b>	5
<b>Vehicle</b>	None

<b>Route of administration</b>	Inhalation
<b>Remarks for test conditions</b>	The respiratory irritation potential of fragrance raw materials was assessed in CD-1 females by recording respiratory rate using a whole body plethysmograph. Mice were exposed to test materials for 1 min using a nebulizer for aerosolization in a 2600 ml chamber. Materials shown to be sensory irritants were further tested in mice cannulated via the trachea & compared to an intact mouse breathing through its nose. Comparisons were between the preexposure & exposure rate values for each material at each dose level. Materials were of undetermined purity.
<b>Value LD50 or LC50 with confidence limits</b>	ED25=590 micrograms/L
<b>Remarks for results</b>	Mild moderate respiratory depression. Lower tract exposures not performed.
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Basic data given and comparable to guidelines/standards.
<b>References</b>	Troy W.R. (1977) Doctoral Dissertation: The comparative respiratory irritation potential of fourteen fragrance raw materials. Unpublished report to RIFM.

<b>Substance Name</b>	Nerol
<b>CAS</b>	106-25-2
<b>Remarks for Substance</b>	Not reported
<b>Method/guideline</b>	NG
<b>Test Type</b>	Acute dermal LD50
<b>GLP</b>	Not reported
<b>Year</b>	1972
<b>Species/Strain</b>	Rabbit/New Zealand White
<b>Sex</b>	Not reported
<b># of animals per sex per dose</b>	10
<b>Vehicle</b>	None
<b>Route of administration</b>	Dermal
<b>Remarks for test conditions</b>	A single 24 hr application was made to the clipped abraded abdominal skin of ten rabbits weighing 1.9 to 2.2 kg. Observations were made for mortality and toxic effects for a period of seven days. Gross necropsies were performed on all animals at the termination of the study.
<b>Value LD50 or LC50 with confidence limits</b>	>5000 mg/kg bw

<b>Number of deaths at each dose level</b>	1 at 5000 mg/kg bw
<b>Remarks for results</b>	The LD50 was reported to be >5000 mg/kg bw.
<b>Conclusion remarks</b>	The LD50 was reported to be >5000 mg/kg bw.
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Basic data given and comparable to guidelines/standards.
<b>References</b>	Moreno O. M. (1972) Acute oral toxicity of nerol in rats and rabbits. Unpublished report to RIFM.

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<b>Substance Name</b>	Nerol
<b>CAS</b>	106-25-2
<b>Remarks for Substance</b>	Clear liquid
<b>Method/guideline</b>	NG
<b>Test Type</b>	Oral LD50
<b>GLP</b>	Not reported
<b>Year</b>	1972
<b>Species/Strain</b>	Rat/Wistar
<b>Sex</b>	Male
<b># of animals per sex per dose</b>	10
<b>Vehicle</b>	None
<b>Route of administration</b>	Oral
<b>Remarks for test conditions</b>	Ten rats per dose level were administered 2560, 4000, 6250 or 9800 mg/kg bw nerol and observed for fourteen days. Gross necropsies performed on all survivors.
<b>Value LD50 or LC50 with confidence limits</b>	4500 mg/kg bw (95% C.L. 3400-5600 mg/kg bw)
<b>Number of deaths at each dose level</b>	2560 mg/kg bw 1/10 deaths; 4000 mg/kg bw 4/10 deaths; 6250 mg/kg bw 7/10 deaths; 9800 mg/kg bw 10/10 deaths
<b>Remarks for results</b>	The animals experienced axophthalmia, hyperreflexiveness, restlessness, lethargy and the loss of the righting reflex. Deaths occurred overnight to two days following administration of the test substance.
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Basic data given and comparable to guidelines/standards.
<b>References</b>	Moreno O. M. (1972) Acute oral toxicity of nerol in rats and rabbits. Unpublished report to RIFM.

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<b>Substance Name</b>	Citral
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<b>CAS</b>	5392-40-5
<b>Remarks for Substance</b>	Substance supported under SIDS.
<b>Method/guideline</b>	Litchfield-Wilcoxon, 1949
<b>Test Type</b>	Oral LD50
<b>GLP</b>	Not reported
<b>Year</b>	1964
<b>Species/Strain</b>	Rat/Osborne-Mendel
<b>Sex</b>	Male and Female
<b># of animals per sex per dose</b>	5
<b>Vehicle</b>	None
<b>Route of administration</b>	Intubation
<b>Remarks for test conditions</b>	5 male and 5 female young adult Osborne-Mendel rats were fasted for 18 hours prior to treatment. Animals were observed for toxic signs and death. The observation period was 2 wks.
<b>Value LD50 or LC50 with confidence limits</b>	4960 mg/kg bw (95% C.L. 3940-6240)
<b>Number of deaths at each dose level</b>	Not reported
<b>Remarks for results</b>	Slope function: 1.5 (95% C.L. 1.2-2.0). Toxic signs were depression. Times of deaths were between 4-96 hours.
<b>Data Qualities Reliabilities</b>	Reliability code 1. Reliable without restrictions.
<b>Remarks for Data Reliability</b>	Guideline study.
<b>References</b>	Jenner P.M., Hagan E.C., Taylor J.M., Cook E.L., Fitzhugh O.G. (1964) Food flavorings and compounds of related structure I. Acute Oral Toxicity. <i>Fd. Cosmet. Toxicol.</i> 2, 327-343.

<b>Substance Name</b>	Acetylated myrcene (data given for major component, geranyl acetate)
<b>CAS</b>	68412-04-4
<b>Remarks for Substance</b>	Principal component of acetylated myrcene
<b>Method/guideline</b>	Litchfield-Wilcoxon, 1949
<b>Test Type</b>	Oral LD50
<b>GLP</b>	Not reported
<b>Year</b>	1964
<b>Species/Strain</b>	Rat/Osborne-Mendel

<b>Sex</b>	Male and Female
<b># of animals per sex per dose</b>	5
<b>Vehicle</b>	None
<b>Route of administration</b>	Intubation
<b>Remarks for test conditions</b>	5 male and 5 female young adult Osborne-Mendel rats were fasted for 18 hours prior to treatment. Animals were observed for toxic signs and death. The observation period was 2 weeks.
<b>Value LD50 or LC50 with confidence limits</b>	6330 mg/kg bw (95% C.L. 5450-7340)
<b>Number of deaths at each dose level</b>	Not reported
<b>Remarks for results</b>	Slope function: 1.3 (95% C.L. 1.2-1.4). Toxic signs were depression. Times of deaths were between 4-96 hours.
<b>Data Qualities Reliabilities</b>	Reliability code 1. Reliable without restrictions.
<b>Remarks for Data Reliability</b>	Guideline study.
<b>References</b>	Jenner P.M., Hagan E.C., Taylor J.M., Cook E.L., Fitzhugh O.G. (1964) Food flavorings and compounds of related structure I. Acute Oral Toxicity. <i>Fd. Cosmet. Toxicol.</i> 2, 327-343.

## 4.2 *In Vitro* Genotoxicity

<b>Substance Name</b>	dl-citronellol
<b>CAS</b>	106-22-9
<b>Method/guideline</b>	Ames
<b>Test Type</b>	Reverse mutation
<b>System of Testing</b>	Bacterial
<b>GLP</b>	No
<b>Year</b>	1979
<b>Species/Strain</b>	Salmonella typhimurium/TA 100 and TA98
<b>Metabolic Activation</b>	Rat liver microsome fraction S9 from Aroclor induced rats
<b>Doses/concentration levels</b>	0.05 - 100 microliters per plate
<b>Statistical Methods</b>	NG
<b>Remarks for test conditions</b>	After 48-hour incubation at 37 °C, each assay plate was counted. Routine positive control plates were prepared: sodium azide & picolonic acid were used as positive controls for TA100 and TA98. Plates with aflatoxin B1 were positive controls for experiments performed with activation by S9

<b>Result</b>	No mutagenic effects
<b>Cytotoxic concentration</b>	NG
<b>Genotoxic effects</b>	None
<b>Statistical evaluations</b>	NG
<b>Conclusion remarks</b>	No evidence of mutagenicity
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Comparable to guideline study with acceptable restrictions. Data were acquired prior to GLP or OECD guidelines but were obtained by standard methodology and published in a peer-reviewed journal.
<b>References</b>	Rockwell P. and Raw I. (1979) A mutagenic screening of various herbs, spices, and food additives. Nutrition and Cancer, 1(4), 10-15.

<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1
<b>Remarks for Substance</b>	99.4% purity
<b>Method/guideline</b>	Chromosomal Aberration test
<b>Test Type</b>	Non-bacterial
<b>System of Testing</b>	Chinese hamster fibroblast
<b>GLP</b>	No
<b>Year</b>	1984
<b>Species/Strain</b>	Chinese hamster fibroblast
<b>Metabolic Activation</b>	None
<b>Doses/concentration levels</b>	3 doses at different concentrations. The maximum dose was 125 ug/plate
<b>Statistical Methods</b>	None performed
<b>Remarks for test conditions</b>	Replicates performed if no dose response was observed. Intervals for testing were 24 and 48 hrs. The solvent used was DMSO. Untreated cells and solvent treated cells were negative controls. The incidence of chromosomal aberrations for negative controls was usually less than 3.0%. 100 metaphases were examined for incidence of aberrations and considered negative <4.9%, equivocal 5.0-9.9%, positive. >10.0%. If no reasonable dose-response relationships were found, additional experiments were conducted at similar dose levels.
<b>Result</b>	Equivocal. Polyploidization effects were observed. The incidence of polyploid cells at 48 hours after treatment was 8.0%. The incidence of chromosomal aberrations at 48 hours was 4.0% at 48 hours.

<b>Cytotoxic concentration</b>	Not given
<b>Genotoxic effects</b>	Polyploidization effects were observed.
<b>Statistical evaluations</b>	Not given
<b>Remarks for results</b>	The result was considered equivocal presumably based on the polyploidization effects observed. The incidence of chromosomal aberrations at 48 hours was in the range considered negative by the authors.
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Test was conducted by standard methodology and published in a peer-reviewed journal. This study closely followed OECD guideline 473, except for metabolic activation and the lack of positive controls.
<b>References</b>	Ishidate M., Sofuni T., Yoshikawa K., Hayashi M., Nohmi T., Sawada M., Matsuoka A. (1984) Primary Mutagenicity Screening of Food Additives Currently Used in Japan. Food Chemical Toxicology. 22, 623-636.

<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1
<b>Remarks for Substance</b>	99.4% purity
<b>Method/guideline</b>	Ames
<b>Test Type</b>	Reverse mutation
<b>System of Testing</b>	Bacterial
<b>GLP</b>	No
<b>Year</b>	1984
<b>Species/Strain</b>	Salmonella typhimurium/TA 92, TA1535, TA100, TA1537, TA94, TA98
<b>Metabolic Activation</b>	With and without rat liver microsome fraction S9 from PCB-induced Fisher rats
<b>Doses/concentration levels</b>	6 different concentrations, maximum tested 500 ug/plate
<b>Statistical Methods</b>	Not given
<b>Remarks for test conditions</b>	DMSO was used as the solvent. Results were considered positive if number of colonies found was at least twice the number found in the control.
<b>Result</b>	Negative
<b>Cytotoxic concentration</b>	Not specified
<b>Genotoxic effects</b>	Negative
<b>Statistical evaluations</b>	Not given
<b>Conclusion remarks</b>	No mutagenic effects

<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Basic data given and comparable to guidelines/standards.
<b>References</b>	Ishidate M., Sofuni T., Yoshikawa K., Hayashi M., Nohmi T., Sawada M., Matsuoka A. (1984) Primary Mutagenicity Screening of Food Additives Currently Used in Japan. Food Chemical Toxicology. 22, 623-636.

<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1
<b>Method/guideline</b>	Ames
<b>Test Type</b>	Reverse mutation
<b>System of Testing</b>	Bacterial
<b>GLP</b>	No
<b>Year</b>	1980
<b>Species/Strain</b>	Salmonella typhimurium/TA 98, TA 100, TA 1535 and TA 1537
<b>Metabolic Activation</b>	With and without rat liver microsome fraction S9 from Aroclor-induced rats
<b>Doses/concentration levels</b>	3 micromol/plate (462 ug/plate)
<b>Statistical Methods</b>	Not given
<b>Remarks for test conditions</b>	The solvent used was ethanol. Only one replicate was performed for the substances, which tested negative.
<b>Result</b>	No mutagenic effects.
<b>Cytotoxic concentration</b>	Not given
<b>Genotoxic effects</b>	None
<b>Statistical evaluations</b>	Not given
<b>Conclusion remarks</b>	No mutagenic activity.
<b>Data Qualities Reliabilities</b>	Reliability code 3. Not reliable.
<b>Remarks for Data Reliability</b>	Does not meet important criteria of today's standard methods.
<b>References</b>	Florin I., Rutberg L., Curvall M., and Enzell C.R. (1980) Screening of tobacco smoke constituents for mutagenicity using the Ames test. Toxicology, 18, 219-232.

<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1
<b>Remarks for Substance</b>	99% purity
<b>Method/guideline</b>	Ames
<b>Test Type</b>	Reverse mutation

<b>System of Testing</b>	Bacterial
<b>GLP</b>	No
<b>Year</b>	1980
<b>Species/Strain</b>	Salmonella typhimurium/TA100
<b>Metabolic Activation</b>	With and without rat liver microsome fraction S9 from Aroclor induced rats
<b>Doses/concentration levels</b>	0.01-1 microliter per 2ml DMSO
<b>Statistical Methods</b>	Not given
<b>Remarks for test conditions</b>	Values are average of two experiments. Positive controls were 6.5 µg sodium azide per 2 ml incubation volume w/out activation and 25 µg 2-aminoanthracene per 2 ml incubation volume with activation. Dose = 0.01 - 1 ul per 2 ml incubation volume in DMSO.
<b>Result</b>	No mutagenic effects
<b>Cytotoxic concentration</b>	Not given
<b>Genotoxic effects</b>	None
<b>Statistical evaluations</b>	Not given
<b>Conclusion remark</b>	No mutagenic activity
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Basic data given and comparable to guidelines/standards.
<b>References</b>	Eder E., Nedecker T., Lutz D., Henschler D. (1980) Mutagenic potential of allyl and allylic compounds. Biochemical Pharmacology 29, 993-998.

<b>Substance Name</b>	Citral
<b>CAS</b>	5392-40-5
<b>Remarks for Substance</b>	Volunteered under SIDS program. 98.2% purity.
<b>Method/guideline</b>	Chromosomal Aberration test
<b>Test Type</b>	Non-bacterial
<b>System of Testing</b>	Chinese hamster fibroblast cell line
<b>GLP</b>	No
<b>Year</b>	1984
<b>Species/Strain</b>	Chinese hamster fibroblast
<b>Metabolic Activation</b>	None
<b>Doses/concentration levels</b>	3 doses at different concentrations. The maximum dose was 30 ug/plate
<b>Statistical Methods</b>	None performed

<b>Remarks for test conditions</b>	Replicates performed if no dose response was observed. Intervals for testing were 24 and 48 hrs. The solvent used was DMSO. Untreated cells and solvent treated cells were negative controls. The incidence of chromosomal aberrations for negative controls was usually less than 3.0%. 100 metaphases were examined for incidence of aberrations and considered negative. <4.9%, equivocal 5.0-9.9%, positive. >10.0%. If no reasonable dose-response relationships were found, additional experiments were conducted at similar dose levels.
<b>Result</b>	Negative. The incidence of polyploid cells at 48 hours after treatment was 4.0%. The incidence of chromosomal aberrations at 48 hours was 2.0%.
<b>Cytotoxic concentration</b>	Not given
<b>Genotoxic effects</b>	Negative
<b>Statistical evaluations</b>	Not given
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Test was conducted by standard methodology and published in a peer-reviewed journal. This study closely followed OECD guideline 473, except for metabolic activation and the lack of positive controls.
<b>References</b>	Ishidate M., Sofuni T., Yoshikawa K., Hayashi M., Nohmi T., Sawada M., Matsuoka A. (1984) Primary Mutagenicity Screening of Food Additives Currently Used in Japan. Food Chemical Toxicology. 22, 623-636.

  

<b>Substance Name</b>	Acetylated myrcene
<b>CAS</b>	68412-04-4
<b>Remarks for Substance</b>	Acetylated myrcene is a mixture that is primarily (62%) acetate esters of nerol and geraniol. Purity of test substance for this assay was 69.6%.
<b>Method/guideline</b>	Ames
<b>Test Type</b>	Reverse mutation
<b>System of Testing</b>	Bacterial
<b>GLP</b>	Not given
<b>Year</b>	1986
<b>Species/Strain</b>	Salmonella typhimurium/TA1535, TA1537, TA97, TA98, TA100
<b>Metabolic Activation</b>	With and without rat and hamster liver microsome fraction S9 from Aroclor-induced rats and hamsters, respectively.
<b>Doses/concentration levels</b>	1-3333 micrograms/plate
<b>Statistical Methods</b>	None employed
<b>Remarks for test conditions</b>	Positive controls included the following: sodium azide for TA1535 and TA100; 4-nitro-o-phenylenediamine for TA98; 9-aminoacridine for TA97 and TA1537; 2-aminoanthracene for all

aminoacridine for TA97 and TA1537; 2-aminoanthracene for all strains with hamster and rat liver metabolic activation. At least 5 dose levels were tested, with 3 plates per dose level. All assays were repeated at least one week following initial assay.

<b>Result</b>	No mutagenic effects.
<b>Cytotoxic concentration</b>	Not given
<b>Genotoxic effects</b>	None
<b>Statistical evaluations</b>	Not given
<b>Conclusion remarks</b>	No evidence of mutagenicity.
<b>Data Qualities Reliabilities</b>	Reliability code 1. Reliable without restrictions.
<b>Remarks for Data Reliability</b>	Guideline study. Test was conducted by laboratory under contract with the National Toxicology Program.
<b>References</b>	Mortelmans, K., Haworth, S., Lawlor, T., Speck, W., Tainer, B., and Zeiger, E. (1986). Salmonella mutagenicity tests: II. Results from the testing of 270 chemicals. Environmental Mutagenesis 8(7), 1-119.

<b>Substance Name</b>	Acetylated myrcene
<b>CAS</b>	68412-04-4
<b>Remarks for Substance</b>	Acetylated myrcene is a mixture that is primarily (62%) acetate esters of nerol and geraniol.
<b>Method/guideline</b>	Ames
<b>Test Type</b>	Reverse mutation
<b>System of Testing</b>	Bacterial
<b>GLP</b>	No
<b>Year</b>	1989
<b>Species/Strain</b>	Salmonella typhimurium/TA1535, TA1537, TA1538, TA98, TA100
<b>Metabolic Activation</b>	Rat liver microsome fraction S9 from Aroclor-induced rats
<b>Doses/concentration levels</b>	20000 ug/plate
<b>Statistical Methods</b>	Not given
<b>Remarks for test conditions</b>	After two days incubation at 37 °C, revertant colonies were counted.
<b>Result</b>	No mutagenic effects.
<b>Cytotoxic concentration</b>	Not given
<b>Genotoxic effects</b>	None
<b>Statistical evaluations</b>	Not given
<b>Conclusion remarks</b>	No evidence of mutagenicity

<b>Data Qualities Reliabilities</b>	Reliability code 1. Reliable without restrictions.
<b>Remarks for Data Reliability</b>	Comparable to guideline study.
<b>References</b>	Heck, J. D., Vollmuth, T. A., Cifone, M. A., Jagannath, D. R., Myhr B., and R.D. Curren (1989). An evaluation of food flavoring ingredients in a genetic toxicity screening battery The Toxicologist, 9(1), 257.

<b>Substance Name</b>	Acetylated myrcene
<b>CAS</b>	68412-04-4
<b>Remarks for Substance</b>	Acetylated myrcene is a mixture that is primarily (62%) acetate esters of nerol and geraniol.
<b>Method/guideline</b>	Unscheduled DNA Synthesis (UDS) Test with Mammalian Liver Cells In Vitro Unscheduled DNA Synthesis
<b>Test Type</b>	Unscheduled DNA Synthesis (Butterworth, 1987)
<b>System of Testing</b>	F344 rat hepatocytes
<b>GLP</b>	No
<b>Year</b>	1989
<b>Species/Strain</b>	Rat/ Adult male Fisher 344
<b>Metabolic Activation</b>	None
<b>Doses/concentration levels</b>	100 nanoliters/millilitre (nl/ml)
<b>Statistical Methods</b>	Not given
<b>Remarks for test conditions</b>	Cultures of freshly prepared hepatocytes were incubated with the test article for 18-20 hours. Cell survival was measured by concurrent cell counting and measurement of LDH release from cells. UDS was measured by counting nuclear grains and subtracting average grain counts in three adjacent nuclear-sized cytoplasmic areas. This was designated the net nuclear grain count (NNG). An NNG in excess of 6 grains was considered a positive response.
<b>Result</b>	No unscheduled DNA synthesis observed.
<b>Cytotoxic concentration</b>	Not given
<b>Genotoxic effects</b>	None
<b>Statistical evaluations</b>	Not given
<b>Conclusion remarks</b>	No evidence of genotoxicity
<b>Data Qualities Reliabilities</b>	Reliability code 1. Reliable without restrictions.
<b>Remarks for Data Reliability</b>	Comparable to guideline study.
<b>References</b>	Heck, J. D., Vollmuth, T. A., Cifone, M. A., Jagannath, D. R., Myhr B., and R.D. Curren (1989). An evaluation of food flavoring ingredients in a genetic toxicity screening battery The Toxicologist, 9(1), 257.

### 4.3 In Vivo Genotoxicity

<b>Substance Name</b>	Acetylated myrcene					
<b>CAS</b>	68412-04-4					
<b>Remarks for Substance</b>	Acetylated myrcene is a mixture that is primarily (62%) acetate esters of nerol and geraniol. The test substance in this study was geranyl acetate (CAS 105-87-3) obtained from the National Toxicology Program Repository. Purity tests revealed the test substance; acetylated myrcene consisted of 79% geranyl acetate and 21% citronellyl acetate. Remaining impurities accounted for less than 0.37%.					
<b>Method/guideline</b>	Mouse bone marrow micronucleus assay					
<b>Test Type</b>	Micronucleus					
<b>GLP</b>	NG					
<b>Year</b>	1993					
<b>Species/Strain</b>	Mouse/ B6C3F1					
<b>Sex</b>	Male					
<b>Route of Administration</b>	Intraperitoneal injection					
<b>Doses/concentration</b>	0, 450, 900, or 1800					
<b>Exposure period</b>	3 days					
<b>Remarks for test conditions</b>	Groups of five to six mice each were administered 0, 450, 900 or 1800 mg/kg bw by intraperitoneal injection for three consecutive days. Positive and negative controls were also maintained. Positive controls were either DMBA (7,12-dimethylbenzanthracene) in corn oil or MMC (mitomycin C) in PBS. 48 hr after the last treatment the mice were euthanized. Bone marrow and peripheral blood smears were obtained by a direct technique					
<b>Effect on mitotic index or PCE/NCE ratio by dose level and sex</b>	Dose	MN-PCE/1000	# Animals	Pairwise Comparison	Survival	PCE
	0	2.20 +/-0.26	5		5/5	65.0
	450	2.50 +/-0.42	5	0.3307	5/5	62.1
	900	3.30+/-1.06	5	0.0687	5/5	66.3
	1800	2.83+/-0.56	6	0.1766	6/6	67.3
<b>Genotoxic effects</b>	Negative					
<b>NOEL (C)/ LOEL (C)</b>	NOEL=1800 mg/kg bw					
<b>Statistical evaluations</b>	Yes, trend test and pairwise comparison alpha=0.05					
<b>Remarks for results</b>	The initial test was negative to the high dose and was not repeated.					
<b>Conclusion</b>	The test was negative.					

<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Basic data given and comparable to guidelines/standards.
<b>References</b>	Shelby M.D., Erexson G.L., Hook G.J., and Tice R.R. (1993) Evaluation of a Three-Exposure Mouse Bone Marrow Micronucleus Protocol; Results with 49 Chemicals. Enviromental and Molecular Mutagenesis, 21: 160-179.
<b>Substance</b>	Acetylated myrcene
<b>CAS</b>	68412-04-4
<b>Remarks for Substance</b>	Acetylated myrcene is a mixture that is primarily (62%) acetate esters of nerol and geraniol.
<b>Method/guideline</b>	Unscheduled DNA Synthesis (UDS) Test with Mammalian Liver Cells In Vivo
<b>Test Type</b>	Unscheduled DNA
<b>GLP</b>	NG
<b>Year</b>	1983
<b>Species/Strain</b>	Rat/Fischer 344
<b>Sex</b>	Male
<b>Route of Administration</b>	Gavage
<b>Genotoxic effects</b>	No genotoxic effects.
<b>Conclusion</b>	No evidence of genotoxicity.
<b>Data Qualities Reliabilities</b>	Reliability code 1. Reliable without restrictions.
<b>Remarks for Data Reliability</b>	Guideline study. Data considered reliable and followed OECD guideline 486. Test was conducted by laboratory under contract with the National Toxicology Program.
<b>References</b>	Mirsalis, J., Tyson, K., Beck, J., Loh, E., Steinmetz, K., Contreras, C., Austere, L., Martin, S., and J. Spalding (1983). Induction of unscheduled DNA synthesis (UDS) in hepatocytes following in vitro and in vivo treatment. Environmental Mutagenesis 5(3), 482.

#### 4.4 Repeat Dose Toxicity

<b>Substance Name</b>	Citronellol
<b>CAS</b>	106-22-9
<b>Remarks for Substance</b>	Mixture of citronellol (50%) and linalool (50%)
<b>Method/guideline</b>	The test mixture was incorporated in the ration at a level designed to provide daily in the food 100 mg of the flavor blend per kg of body wt. The un-supplemented diet was fed to the controls. The rats were fed for 12 weeks

<b>GLP</b>	Pre-GLP
<b>Year</b>	1958
<b>Species/Strain</b>	Unspecified strain rat
<b>Sex</b>	Male and Female
<b>Route of administration</b>	Diet
<b>Doses/concentration levels</b>	100 mg/kg of mixture per day
<b>Exposure period</b>	12 weeks
<b>Frequency of treatment</b>	Continuously in diet
<b>Control Group</b>	Yes
<b>Post exposure observation period</b>	NG
<b>Remarks for test conditions</b>	After 12 weeks on test, the urine of 3 rats of each sex per group was examined for the presence of sugar and albumin, blood hemoglobin levels were determined and autopsies were performed on all animals.
<b>NOAEL(NOEL)</b>	100 mg/kg bw/day ppm
<b>LOAEL(LOEL)</b>	No adverse effects at highest dose
<b>Actual dose received by dose level and sex</b>	Not given
<b>Toxic response/effects by dose level</b>	No adverse effects on efficiency of food utilization or other observable physiological criteria were noted.
<b>Statistical evaluations</b>	Not given
<b>Remarks for results</b>	The depression in the growth and food intake of the male rats was attributed to impalatibility of the test material at the level administered.
<b>Conclusion remarks</b>	Feeding tests with a mixture of equal parts of citronellol and linalool fed at a level 100 times the estimated use level in the diet disclosed no adverse effect on efficiency of food utilization or other observable criteria..
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>References</b>	Oser, B. (1958) Toxicological Screening of Components of Food Flavors Class VI. Citronellol and Linalool. Food and Drug Research Laboratories.

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<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1
<b>Remarks for Substance</b>	Mixture of 3,7-dimethyl-2,6-octadienol (geraniol) and 3,7-dimethyl-6-octenol (citronellol)

<b>Method/guideline</b>	Screening method used by U.S. Food and Drug Administration
<b>GLP</b>	No
<b>Year</b>	1967
<b>Species/Strain</b>	Osborne-Mendel rats
<b>Sex</b>	Male and Female
<b>Route of administration</b>	Diet
<b>Doses/concentration levels</b>	1000 or 10000 ppm
<b>Exposure period</b>	112 days at 10,000 ppm, 189-196 days at 1000 ppm
<b>Frequency of treatment</b>	Continuously in diet
<b>Control Group</b>	Yes
<b>Post exposure observation period</b>	NG
<b>Remarks for test conditions</b>	Groups of five male and five female Osborne-Mendel rats were provided geraniol in the diet at concentrations of 0, 1000 or 10,000 ppm for 16 and 27-28 weeks, respectively. No vehicle was used. The diet was prepared and analyzed weekly. Measurements of body weight, food intake and general condition were recorded weekly. Hematological examinations (white cell counts, red cell counts, hemoglobins and hematocrits) were performed at the termination of the study. Macroscopic examination of all tissues was performed. Histopathological examination was performed on the liver, kidneys, spleen, heart, and testes of 6-8 animals (evenly divided by sex) from both doses and the control dose group.
<b>NOAEL(NOEL)</b>	10000 ppm
<b>LOAEL(LOEL)</b>	No adverse effects at highest dose
<b>Actual dose received by dose level and sex</b>	Not given
<b>Toxic response/effects by dose level</b>	None
<b>Statistical evaluations</b>	Not given
<b>Remarks for results</b>	Measurements of body weight, food intake and general condition recorded weekly showed no significant differences between test and control animals at any intake level. At termination, hematological examinations revealed no difference from controls. At necropsy, no differences were reported between major organ weights of test and control animals. Gross examination of tissue of all animals was unremarkable and histopathological examination revealed no treatment-related lesions.
<b>Conclusion remarks</b>	This study demonstrates a NOAEL in rats of at least 500 mg/kg/day.

<b>Data Qualities Reliabilities</b>	Reliability code 1. Reliable without restrictions.
<b>Remarks for Data Reliability</b>	Comparable to guideline study. This study was performed by the FDA prior to the establishment of GLP and OECD.
<b>References</b>	Hagan E.C., Hansen W.H., Fitzhugh O.G., Jenner P.M., Jones W.I., Taylor J.M., Long E.L., Nelson A.A., and Brouwer J.B. (1967) Food Flavours and Compounds of Related Structure. II. Subacute and Chronic Toxicity. Food Cosmetic Toxicology 5, 141-157.

<b>Substance Name</b>	Citral
<b>CAS</b>	5392-40-5
<b>Remarks for Substance</b>	Substance supported under SIDS.
<b>Method/guideline</b>	Screening method used by U.S. Food and Drug Administration.
<b>GLP</b>	No
<b>Year</b>	1967
<b>Species/Strain</b>	Osborne-Mendel rats
<b>Sex</b>	Male and Female
<b>Route of administration</b>	Diet
<b>Doses/concentration levels</b>	1000, 2500 or 10000 ppm
<b>Exposure period</b>	91 days
<b>Frequency of treatment</b>	Continuously in diet
<b>Control Group</b>	Yes
<b>Post exposure observation period</b>	Not given
<b>Remarks for test conditions</b>	Groups of ten male and ten female Osborne-Mendel rats were provided citral in the diet at concentrations of 0, 1000, 2500 or 10,000 ppm for 13 weeks. No vehicle was used. The diet was prepared and analyzed weekly. Measurements of body weight, food intake and general condition were recorded weekly. Hematological examinations (white cell counts, red cell counts, hemoglobins and hematocrits) were performed at the termination of the study. Macroscopic examination of all tissues was performed. Histopathological examination was performed on the liver, kidneys, spleen, heart, and testes of 6-8 animals (evenly divided by sex) from the high dose and control dose groups.
<b>NOAEL(NOEL)</b>	10000 ppm
<b>LOAEL(LOEL)</b>	No adverse effects at highest dose
<b>Actual dose received by dose level and sex</b>	Not given
<b>Toxic response/effects by dose level</b>	None.

<b>dose level</b>	
<b>Statistical evaluations</b>	Not given
<b>Remarks for results</b>	Determination of the dietary concentration of citral revealed a weekly loss of 58% therefore the average daily dose received is estimated to be about 200 mg/kg based on an assumed daily intake of food of 50g/kg. Measurements of body weight, food intake and general condition recorded weekly showed no significant differences between test and control animals at any intake level. At termination, hematological examinations revealed no difference from controls. At necropsy, no differences were reported between major organ weights of test and control animals. Gross examination of tissue of all animals was unremarkable and histopathological examination revealed no treatment-related lesions.
<b>Conclusion remarks</b>	This study demonstrates a NOAEL in rats of at least 200 mg/kg/day.
<b>Data Qualities Reliabilities</b>	Reliability code 1. Reliable without restrictions.
<b>Remarks for Data Reliability</b>	Comparable to guideline study. This study was performed by the FDA prior to the establishment of GLP and OECD.
<b>References</b>	Hagan E.C., Hansen W.H., Fitzhugh O.G., Jenner P.M., Jones W.I., Taylor J.M., Long E.L., Nelson A.A., and Brouwer J.B. (1967) Food Flavourings and Compounds of Related Structure. II. Subacute and Chronic Toxicity. Food Cosmetic Toxicology 5, 141-157.

<b>Substance Name</b>	Acetylated myrcene
<b>CAS</b>	68412-04-4
<b>Remarks for Substance</b>	Acetylated myrcene is a mixture that is primarily (62%) acetate esters of nerol and geraniol. The test substance under study is geranyl acetate (CAS 105-87-3).
<b>Method/guideline</b>	Screening method used by U.S. Food and Drug Administration
<b>GLP</b>	Not given
<b>Year</b>	1967
<b>Species/Strain</b>	Osborne-Mendel rats
<b>Sex</b>	Male and Female
<b>Route of administration</b>	Diet
<b>Doses/concentration levels</b>	1000, 2500 or 10000 ppm
<b>Exposure period</b>	118 days
<b>Frequency of treatment</b>	Continuously in diet
<b>Control Group</b>	Yes
<b>Post exposure observation period</b>	Not given
<b>Remarks for test conditions</b>	Groups of ten male and ten female Osborne-Mendel rats were

provided geranyl acetate in the diet at concentrations of 0, 1000, 2500 or 10,000 ppm for 17 weeks. No vehicle was used. The diet was prepared and analyzed weekly. Measurements of body weight, food intake and general condition were recorded weekly. Hematological examinations (white cell counts, red cell counts, hemoglobins and hematocrits) were performed at the termination of the study. Macroscopic examination of all tissues was performed. Histopathological examination was performed on the liver, kidneys, spleen, heart, and testes of 6-8 animals (evenly divided by sex) from the high dose and control dose groups.

<b>NOAEL(NOEL)</b>	10000 ppm
<b>LOAEL(LOEL)</b>	No adverse effects at highest dose
<b>Actual dose received by dose level and sex</b>	Not given
<b>Toxic response/effects by dose level</b>	None.
<b>Statistical evaluations</b>	Not given
<b>Remarks for results</b>	Determination of the dietary concentration of geranyl acetate revealed a weekly loss of 4%. The average daily dose received is estimated to be about 500 mg/kg based on an assumed daily intake of food of 50g/kg. Measurements of body weight, food intake and general condition recorded weekly showed no significant differences between test and control animals at any intake level. At termination, hematological examinations revealed no difference from controls. At necropsy, no differences were reported between major organ weights of test and control animals. Gross examination of tissue of all animals was unremarkable and histopathological examination revealed no treatment-related lesions.
<b>Conclusion remarks</b>	This study demonstrates a NOAEL in rats of at least 500 mg/kg/day.
<b>Data Qualities Reliabilities</b>	Reliability code 1. Reliable without restrictions.
<b>Remarks for Data Reliability</b>	Comparable to guideline study. This study was performed by the FDA prior to the establishment of GLP and OECD.
<b>References</b>	Hagan E.C., Hansen W.H., Fitzhugh O.G., Jenner P.M., Jones W.I., Taylor J.M., Long E.L., Nelson A.A., and Brouwer J.B. (1967) Food Flavours and Compounds of Related Structure. II. Subacute and Chronic Toxicity. Food Cosmetic Toxicology 5, 141-157.

<b>Substance Name</b>	Acetylated myrcene
<b>CAS</b>	68412-04-4
<b>Remarks for Substance</b>	Acetylated myrcene is a mixture that is primarily (62%) acetate esters of nerol and geraniol. The test substance was food grade geranyl acetate (CAS 105-87-3). Purity tests revealed the test

	geranyl acetate (CAS 105-87-3). Purity tests revealed the test substance consisted of 79% geranyl acetate and 29% citronellyl acetate. Remaining impurities accounted for less than 0.37%.
<b>Method/guideline</b>	National Toxicology Program Carcinogenesis study (NIH Publication No. 88-2508) or (NTP TR 252).
<b>GLP</b>	Yes
<b>Year</b>	1987
<b>Species/Strain</b>	F344/N rats
<b>Sex</b>	Male and Female
<b>Route of administration</b>	Gavage
<b>Doses/concentration levels</b>	1000 or 2000 mg/kg bw/d
<b>Exposure period</b>	103 weeks
<b>Frequency of treatment</b>	Daily (5 days/week)
<b>Control Group</b>	Yes
<b>Post exposure observation period</b>	Not given
<b>Remarks for test conditions</b>	A carcinogenicity study was conducted in which groups of 50 F344/N rats of each sex were administered 0, 1000, or 2000 mg/kg bw of a mixture of geranyl acetate (79%) and citronellyl acetate (29%) in corn oil by gavage daily, 5 days/week for 103 weeks. Body weights were recorded weekly for the first 12 weeks and monthly thereafter. Necropsies were performed on all animals surviving until the end of the study and on all animals found dead during the study. Histopathological examination was conducted on the following: gross lesions, tissue masses, abnormal lymph nodes, skin, mandibular lymph nodes, mammary gland, salivary gland, thigh muscle, sciatic nerve, bone marrow, thymus, larynx, trachea, lungs, and bronchi, heart, thyroid, parathyroid, esophagus, stomach, duodenum, jejunum, ileum, colon, mesenteric lymph nodes, liver, pancreas, spleen, kidneys, adrenals, urinary bladder, seminal vesicles/prostate/testes or ovaries/uterus, brain, pituitary, and spinal cord.
<b>NOAEL(NOEL)</b>	2000 mg/kg bw/d
<b>Actual dose received by dose level and sex</b>	Not applicable
<b>Toxic response/effects by dose level</b>	A statistically significant decrease in mean body weights was reported for high-dose male rats throughout the study and dosed female rats after week 40. Reduced mean body weight gains were dose related. Survival of the high-dose group (18/50) of male rats was significantly less than the controls (34/50; $p=0.001$ ) and the low-dose group (29/50; $p=0.003$ ). There was no other significant difference in survival between any groups of either sex. There was a statistically significant ( $p<0.05$ ) increase in the incidence of squamous cell neoplasms (combined papillomas and carcinomas) in low-dose male rats, but not in the high-dose group (controls, 0/50; low dose, 5/50;

but not in the high-dose group (controls, 0/50; low dose, 5/50; high dose, 1/50) or any group of female rats. A positive trend (controls, 6/50; low dose, 8/50; high dose, 9/50) in the incidence of adrenal pheochromocytomas in male rats was not statistically significant. Two (2) low-dose male rats had tubular cell adenomas, but none were observed in the controls or the high-dose group. There was no significant increase in the incidence of any neoplasms in high-dose male or female rats compared to the control groups. The incidence of mammary gland fibroadenomas in high-dose female rats was significantly less (pairwise comparisons,  $p < 0.002$ ) than those in the control group (controls, 12/50; high dose, 1/50). Based on pair-wise comparisons between high-dose and control groups of male rats, there was a significant decrease ( $p < 0.02$ , Fisher) in the incidence of pituitary adenomas in high-dose males (controls, 10/50; high dose, 2/50). Based on life table analysis of male rats, the incidence of adenomas was not significantly different between control and high-dose groups. A negative trend (controls, 4/49; low dose, 3/48; high dose, 0/50) was observed in the incidence of pancreatic islet-cell adenomas and carcinomas in male rats, but was not statistically significant based on pairwise comparisons between control and dosed groups.

#### Statistical evaluations

Not given

#### Remarks for results

A statistically significant decrease in mean body weights was reported for high-dose male rats throughout the study and dosed female rats after week 40. Reduced mean body weight gains were dose related. Survival of the high-dose group (18/50) of male rats was significantly less than the controls (34/50;  $p = 0.001$ ) and the low-dose group (29/50;  $p = 0.003$ ). There was no other significant difference in survival between any groups of either sex. There was a statistically significant ( $p < 0.05$ ) increase in the incidence of squamous cell neoplasms (combined papillomas and carcinomas) in low-dose male rats, but not in the high-dose group (controls, 0/50; low dose, 5/50; high dose, 1/50) or any group of female rats. A positive trend (controls, 6/50; low dose, 8/50; high dose, 9/50) in the incidence of adrenal pheochromocytomas in male rats was not statistically significant. Two (2) low-dose male rats had tubular cell adenomas, but none were observed in the controls or the high-dose group. There was no significant increase in the incidence of any neoplasms in high-dose male or female rats compared to the control groups. The incidence of mammary gland fibroadenomas in high-dose female rats was significantly less (pairwise comparisons,  $p < 0.002$ ) than those in the control group (controls, 12/50; high dose, 1/50). Based on pair-wise comparisons between high-dose and control groups of male rats, there was a significant decrease ( $p < 0.02$ , Fisher) in the incidence of pituitary adenomas in high-dose males (controls, 10/50; high dose, 2/50). Based on life table analysis of male rats, the incidence of adenomas was not significantly different between control and high-dose groups. A negative trend (controls, 4/49; low dose, 3/48; high dose, 0/50) was observed in the incidence of pancreatic islet-cell adenomas and carcinomas in male rats, but was not statistically significant

	<p>based on pairwise comparisons between control and dosed groups [NTP, 1987]. The increases in the incidence of squamous cell papillomas and carcinomas, adrenal pheochromocytomas, and renal tubular adenomas in male rats were not dose related. These types of tumors occur commonly in male F344 rats. The overall incidence of these commonly observed adrenal pheochromocytomas and squamous cell tumors in paired control groups of male rats have been reported to be 25.1% and 3.7%, respectively [Haseman et al., 1986]. Under conditions of this study, geranyl acetate was not carcinogenic for either sex of F344/N rats [NTP, 1987]. In summary, no significant toxic or carcinogenic effects were reported when a mixture of geranyl acetate and citronellyl acetate was administered at dose levels up to 2000 mg/kg bw/d to rats, which correspond to estimated dose levels of 1420 mg geranyl acetate/kg bw/d and 580 mg citronellyl acetate/kg bw/d (the estimated dose levels correspond to 71% and 29% of the administered dose which are the fractions of geranyl acetate and citronellyl acetate contained in the mixture).</p>
<b>Conclusion remarks</b>	Under conditions of this study, the mixture of geranyl acetate and citronellyl acetate was not carcinogenic for either sex of B6C3F1 mice.
<b>Data Qualities Reliabilities</b>	Reliability code 1. Reliable without restrictions.
<b>Remarks for Data Reliability</b>	Guideline study. This study was performed by the NTP.
<b>References</b>	National Toxicology Program (NTP) (1987) Carcinogenesis studies of food grade geranyl acetate (71%) and citronellyl acetate (29%). NTP-TR-252. National Technical Information Services. PB-88-2508.

<b>Substance Name</b>	Acetylated myrcene
<b>CAS</b>	68412-04-4
<b>Remarks for Substance</b>	Acetylated myrcene is a mixture that is primarily (62%) acetate esters of nerol and geraniol. The test substance in this study was food grade geranyl acetate (CAS 105-87-3). Purity tests revealed the test substance consisted of 79% geranyl acetate and 29% citronellyl acetate. Remaining impurities accounted for less than 0.37%.
<b>Method/guideline</b>	National Toxicology Program Carcinogenesis study (NIH Publication No. 88-2508) or (NTP TR 252).
<b>GLP</b>	Yes
<b>Year</b>	1987
<b>Species/Strain</b>	Mouse/B6C3F1
<b>Sex</b>	Male and Female
<b>Route of administration</b>	Gavage
<b>Doses/concentration levels</b>	500 or 1000 mg/kg bw/d
<b>Exposure period</b>	103 weeks
<b>Frequency of treatment</b>	Daily (5 days/week)

<b>Control Group</b>	Yes
<b>Post exposure observation period</b>	Not given
<b>Remarks for test conditions</b>	A carcinogenicity study was conducted in which groups of 50 B6C3F1 mice of each sex were administered 0, 500, or 1000 mg/kg bw of a mixture of geranyl acetate (79%) and citronellyl acetate (29%) in corn oil by gavage daily, 5 days/week for 103 weeks. Body weights were recorded weekly for the first 12 weeks and monthly thereafter. Necropsies were performed on all animals surviving until the end of the study and on all animals found dead during the study. Histopathological examination was conducted on the following: gross lesions, tissue masses, abnormal lymph nodes, skin, mandibular lymph nodes, mammary gland, salivary gland, thigh muscle, sciatic nerve, bone marrow, thymus, larynx, trachea, lungs, and bronchi, heart, thyroid, parathyroid, esophagus, stomach, duodenum, jejunum, ileum, colon, mesenteric lymph nodes, liver, gallbladder, pancreas, spleen, kidneys, adrenals, urinary bladder, seminal vesicles/prostate/testes or ovaries/uterus, brain, pituitary, and spinal cord.
<b>NOAEL(NOEL)</b>	1000 mg/kg bw/d
<b>LOAEL(LOEL)</b>	>1000 mg/kg bw/d
<b>Actual dose received by dose level and sex</b>	Not applicable
<b>Toxic response/effects by dose level</b>	<p>Mean body weights of high-dose male and female mice were lower than those of control groups after week 18 of the study. Survival of male mice in the high-dose group was significantly reduced (controls, 31/50; high dose, 0/50). Survival of the high- and low-dose groups of female mice was significantly less (<math>p&lt;0.001</math>; low dose, 0.020) than that of the control group (controls, 28/50; low dose, 15/50; high dose, 0/50).</p> <p>Inflammation of the vagina, uterus, ovaries, or multiple organs occurred in 18 control, 14 low-dose, and 2 high-dose female mice. The incidence of malignant lymphoma in high-dose male mice was significantly less (<math>p&lt;0.044</math>) than in the control group (controls, 7/50; high dose, 1/50). There was a significant (<math>p=0.030</math>, Fisher) decrease in the incidence of thyroid follicular-cell adenoma in high dose female mice (controls, 7/50; high dose, 1/50). The incidence of non-neoplastic lesions was significantly increased in high-dose male and female mice only; an increased incidence of cytoplasmic vacuolization of the liver in male (control, 1/50; low dose, 7/50; high dose, 47/50) and female mice (control, 1/50; low dose, 27/50; high dose, 46/50) and the kidney or kidney tubule in male (control, 0/50; low dose, 0/50; high dose, 41/50) and female mice (control, 0/50; low dose, 24/49; high dose, 37/50).</p>
<b>Statistical evaluations</b>	Not given
<b>Remarks for results</b>	The probable cause of death of many females was a genital tract infection. Inflammation of the vagina, uterus, ovaries, or multiple organs occurred in 18 control, 14 low-dose, and 2 high-dose female mice. Although the etiologic agent was not isolated, Klebsiella pneumoniae were isolated from similarly affected mice at this laboratory in subsequent chronic studies. Surviving male (36) and female (11) mice in the high-dose

	<p>Surviving male (36) and female (11) mice in the high-dose groups were killed in a moribund condition at week 91 after an inadvertent overdose of the test substance. Eleven other animals (3 control males, 3 low-dose males, 3 low-dose females and 2 high-dose females) were killed by gavage accidents during the course of the study. There was no increase in the incidence of neoplastic lesions associated with administration of the test substance. The incidence of non-neoplastic lesions was significantly increased in high-dose male and female mice only; an increased incidence of cytoplasmic vacuolization of the liver in male (control, 1/50; low dose, 7/50; high dose, 47/50) and female mice (control, 1/50; low dose, 27/50; high dose, 46/50) and the kidney or kidney tubule in male (control, 0/50; low dose, 0/50; high dose, 41/50) and female mice (control, 0/50; low dose, 24/49; high dose, 37/50).</p>
<b>Conclusion remarks</b>	Under conditions of this study, the mixture of geranyl acetate and citronellyl acetate was not carcinogenic for either sex of B6C3F1 mice.
<b>Data Qualities Reliabilities</b>	Reliability code 1. Reliable without restrictions.
<b>Remarks for Data Reliability</b>	Guideline study. This study was performed by the NTP.
<b>References</b>	National Toxicology Program (NTP) (1987) Carcinogenesis studies of food grade geranyl acetate (71%) and citronellyl acetate (29%). NTP-TR-252. National Technical Information Services. PB-88-2508.

<b>Substance Name</b>	Acetylated myrcene
<b>CAS</b>	68412-04-4
<b>Remarks for Substance</b>	Acetylated myrcene is a mixture that is primarily (62%) acetate esters of nerol and geraniol. The test substance in this study was food grade geranyl acetate (CAS 105-87-3). Purity tests revealed the test substance consisted of 79% geranyl acetate and 29% citronellyl acetate. Remaining impurities accounted for less than 0.37%.
<b>Method/guideline</b>	National Toxicology Program Carcinogenesis study (NIH Publication No. 88-2508) or (NTP TR 252).
<b>GLP</b>	Yes
<b>Year</b>	1987
<b>Species/Strain</b>	B6C3F1 mice
<b>Sex</b>	Male and Female
<b>Route of administration</b>	Gavage
<b>Doses/concentration levels</b>	125, 250, 500, 1000, or 2000 mg/kg bw/d
<b>Exposure period</b>	13 weeks
<b>Frequency of treatment</b>	Daily (5 days/week)
<b>Control Group</b>	Yes

<b>Post exposure observation period</b>	Not given
<b>Remarks for test conditions</b>	In a 13-week study, a mixture of geranyl acetate (71%) and citronellyl acetate (29%) was administered by gavage in corn oil to six groups of B6C3F1 mice (10/sex/group) at dose levels of 0, 125, 250, 500, 1000, or 2000 mg/kg bw daily 5 days/week. Animals were checked twice daily for mortality and signs of morbidity. Body weight data were collected weekly. Necropsies were performed on all animals surviving until the end of the study and on all animals found dead during the study. Histopathologic examination was conducted on the following organs for the 2000 mg/kg bw/d dose group and the control groups: gross lesions, tissue masses, abnormal lymph nodes, skin, mandibular lymph nodes, mammary gland, salivary gland, thigh muscle, sciatic nerve, bone marrow, thymus, larynx, trachea, lungs, and bronchi, heart, thyroid, parathyroid, esophagus, stomach, duodenum, jejunum, ileum, colon, mesenteric lymph nodes, liver, gallbladder, pancreas, spleen, kidneys, adrenals, urinary bladder, seminal vesicles/prostate/testes or ovaries/uterus, brain, pituitary, and spinal cord.
<b>NOAEL(NOEL)</b>	1000 mg/kg bw/d
<b>LOAEL(LOEL)</b>	2000 mg/kg bw/d
<b>Actual dose received by dose level and sex</b>	NA
<b>Toxic response/effects by dose level</b>	Seven (7) of 10 males and 9/10 females receiving 2000 mg/kg bw/d died during the study. Male and female mice in the 2000 mg/kg bw/d dose groups exhibited cytoplasmic vacuolization of the liver, kidney and myocardium.
<b>Statistical evaluations</b>	Not given
<b>Remarks for results</b>	Gavage errors resulted in the death of three females at lower dose levels. Mean body weights were comparable for dosed and control animals. Male and female mice in the 2000 mg/kg bw/d dose groups exhibited cytoplasmic vacuolization of the liver, kidney and myocardium. Vacuolization was the result of lipid droplets that were present throughout the liver lobule, particularly in the periportal region. No treatment-related histopathological lesions or other effects were observed in the 1000 mg/kg bw/d group.
<b>Conclusion remarks</b>	This study demonstrates a NOAEL in mice of 1000 mg/kg bw/day.
<b>Data Qualities Reliabilities</b>	Reliability code 1. Reliable without restrictions.
<b>Remarks for Data Reliability</b>	Guideline study. This study was performed by the NTP.
<b>References</b>	National Toxicology Program (NTP) (1987) Carcinogenesis studies of food grade geranyl acetate (71%) and citronellyl acetate (29%). NTP-TR-252. National Technical Information Services. PB-88-2508.

<b>Substance Name</b>	Acetylated myrcene
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<b>CAS</b>	68412-04-4
<b>Remarks for Substance</b>	Acetylated myrcene is a mixture that is primarily (62%) acetate esters of nerol and geraniol. The test substance in this study was food grade geranyl acetate (CAS 105-87-3). Purity tests revealed the test substance consisted of 79% geranyl acetate and 29% citronellyl acetate. Remaining impurities accounted for less than 0.37%.
<b>Method/guideline</b>	National Toxicology Program Carcinogenesis study (NIH Publication No. 88-2508) or (NTP TR 252).
<b>GLP</b>	Yes
<b>Year</b>	1987
<b>Species/Strain</b>	Rat/F344/N
<b>Sex</b>	Male and Female
<b>Route of administration</b>	Gavage
<b>Doses/concentration levels</b>	250, 500, 1000, 2000 or 4000 mg/kg bw/d
<b>Exposure period</b>	13 weeks
<b>Frequency of treatment</b>	Daily (5 days/week)
<b>Control Group</b>	Yes
<b>Post exposure observation period</b>	NG
<b>Remarks for test conditions</b>	In a 13-week study, a mixture of geranyl acetate (71%) and citronellyl acetate (29%) was administered by gavage in corn oil to six groups of F344/N rats (10/sex/group) at dose levels of 0, 125, 250, 500, 1000, or 2000 mg/kg bw daily 5 days/week. Animals were checked twice daily for mortality and signs of morbidity. Body weight data were collected weekly. Necropsies were performed on all animals surviving until the end of the study and on all animals found dead during the study. Histopathologic examination was conducted on the following organs for the 2000 mg/kg bw/d dose group and the control groups: gross lesions, tissue masses, abnormal lymph nodes, skin, mandibular lymph nodes, mammary gland, salivary gland, thigh muscle, sciatic nerve, bone marrow, thymus, larynx, trachea, lungs, and bronchi, heart, thyroid, parathyroid, esophagus, stomach, duodenum, jejunum, ileum, colon, mesenteric lymph nodes, liver, pancreas, spleen, kidneys, adrenals, urinary bladder, seminal vesicles/prostate/testes or ovaries/uterus, brain, pituitary, and spinal cord.
<b>NOAEL(NOEL)</b>	2000 mg/kg bw/d
<b>LOAEL(LOEL)</b>	4000 mg/kg bw/d
<b>Actual dose received by dose level and sex</b>	NA
<b>Toxic response/effects by dose level</b>	Two of ten males and 1/10 females receiving 4000 mg/kg bw/d died. A decrease in mean body weight gain in males and females (19 % and 8% relative to controls, respectively) was reported at the 4000 mg/kg bw/d dose level.

reported at the 4000 mg/kg bw/d dose level.

<b>Statistical evaluations</b>	Not given
<b>Remarks for results</b>	Mean body weights were comparable for dosed and control animals, except for a decrease in mean body weight gain in males and females (19 % and 8% relative to controls, respectively) at the 4000 mg/kg bw/d dose level. No treatment-related histopathologic effects were observed at necropsy.
<b>Conclusion remarks</b>	This demonstrates a NOAEL in rats of 2000 mg/kg bw/day.
<b>Data Qualities Reliabilities</b>	Reliability code 1. Reliable without restrictions.
<b>Remarks for Data Reliability</b>	Guideline study. This study was performed by the NTP.
<b>References</b>	National Toxicology Program (NTP) (1987) Carcinogenesis studies of food grade geranyl acetate (71%) and citronellyl acetate (29%). NTP-TR-252. National Technical Information Services. PB-88-2508.

## 4.5 Reproductive Toxicity

<b>Substance Name</b>	Citral (Mixture of geranial and neral)
<b>CAS</b>	5392-40-5
<b>Remarks for Substance</b>	Volunteered under SIDS program.
<b>Method/guideline</b>	Not given
<b>Test Type</b>	Two generation
<b>GLP</b>	Not given
<b>Year</b>	1989
<b>Species/Strain</b>	Rat/ CR Sprague Dawley
<b>Sex</b>	Female
<b>Route of administration</b>	Oral
<b>Duration of test</b>	14 days prior to cohabitation; days 0 through 25 of presumed gestation; days 1-21 of lactation
<b>Doses/concentration levels</b>	50, 160, 500 mg/kg bw/d
<b>Premating Exposure period for males</b>	Not available
<b>Premating Exposure period for females</b>	14 days
<b>Frequency of treatment</b>	Continuous
<b>Control Group and treatment</b>	Yes
<b>Remarks for test conditions</b>	Thirty Sprague/Dawley/Charles River females rats were administered citral at dose levels of 0, 50, 160, and 500 mg/kg bw/d for 14 days prior to cohabitation, days 0-25 of presumed gestation and days 1-21 of lactation. Per group, fifteen rats were assigned to caesarean sectioning while the other fifteen were assigned natural delivery. Parameters evaluated for the

	were assigned natural delivery. Parameters evaluated for the adult female rats included clinical observation, estrous cycle, body weight and body weight change, feed consumption, mating and fertility, duration of gestation, delivery and maternal behavior, reproductive indices, and gross necropsy. Fetuses were evaluated for fetal wastage, body weight, sex and gross external examination. Pups were evaluated for clinical observations, body weight and gross necropsy.
<b>NOAEL(NOEL)</b>	50 mg/kg bw/d
<b>LOAEL(LOEL)</b>	160 mg/kg bw/d
<b>Actual dose received by dose level and sex</b>	Not available
<b>Parental data and F1 as appropriate</b>	At the 160 and 500 mg/kg bw/d dose levels, increased mortality (1/30 and 7/30, respectively), clinical signs of toxicity, significant decreases in body weight gain during gestation, and significant increases in feed consumption during lactation. No adverse effects were reported on estrous cycling, mating, fertility, duration of gestation, numbers of corpora lutea, number of implantations, live litter sizes, resorption of male/female ratio at dosages as high as 500 mg/kg bw/d.
<b>Offspring toxicity F1 and F2</b>	Decreases in fetal body weight (not statistically significant) were reported for fetuses delivered by Cesarean delivery, and significantly decreased pup body weight for delivered pups were reported at the 500 mg/kg bw/d level. No other effects were reported in the offspring.
<b>Statistical evaluations</b>	Yes, ANOVA F test
<b>Remarks for results</b>	The maternal NOAEL is 50 mg/kg bw/d and the fetal/pup NOAEL is 160 mg/kg bw/d.
<b>Conclusion remarks</b>	Citral did not affect the reproductive performance or the pre-weaning development of offspring in female Sprague/Dawley Charles River female rats.
<b>Data Qualities Reliabilities</b>	Reliability code 1. Reliable without restrictions.
<b>Remarks for Data Reliability</b>	Comparable to guideline study.
<b>References</b>	Hoberman, A.M., Christian, M.S., Bennett, M.B. and Vollmuth, T.A. (1989). Abstract. Oral general reproduction study of citral in female rats. The Toxicologist 9, 271.

#### 4.6 Developmental/Teratogenicity Toxicity

<b>Substance Name</b>	Geraniol
<b>CAS</b>	106-24-1
<b>Remarks for Substance</b>	The test substance was citral diethyl acetal, the diethyl acetal of geranial.
<b>Method/guideline</b>	<i>In vivo</i> Reproductive and Developmental Tox. Screening Test

<b>Test Type</b>	<i>In vivo</i> mammalian test system
<b>GLP</b>	No
<b>Year</b>	1997
<b>Species/Strain</b>	Rat/Sprague Dawley
<b>Sex</b>	Female
<b>Route of administration</b>	Oral
<b>Duration of test</b>	39 days
<b>Doses/concentration levels</b>	0, 125, 250, 500 mg/kg bw/d
<b>Exposure period</b>	14 days
<b>Frequency of treatment</b>	Daily
<b>Control Group and treatment</b>	Vehicle alone
<b>Remarks for test conditions</b>	The test substance was administered orally by gavage at the dose levels specified or the vehicle alone for seven days prior to cohabitation and then through cohabitation, gestation, delivery and a 4-day lactation/postparturation period. The vehicle was either corn oil or methylcellulose. Body weights, food consumption and clinical signs were recorded throughout the observation period. All dams were necropsied and examined for gross lesions on Day 25 of presumed gestation for rats not delivering a litter and four days postpartum for rats delivering a litter. Pups delivered were sacrificed on day 4 postpartum, any pups dying during the lactation period were necropsied.
<b>NOAEL(NOEL) maternal</b>	125 mg/kg bw/d
<b>LOAEL(LOEL) maternal</b>	250 mg/kg bw/d
<b>NOAEL (NOEL) developmental</b>	250 mg/kg bw/d
<b>LOAEL (LOEL) developmental</b>	500 mg/kg bw/d
<b>Actual dose received by dose level and sex</b>	Not given
<b>Maternal data with dose level</b>	125 mg/kg bw/d- no effects; 250 mg/kg bw/d-clinical observations, body weight decrease compared to control, reduced body weight gain compared to control; 500 mg/kg bw/d-clinical observations, body weight decrease compared to control, reduced body weight gain compared to control
<b>Fetal data with dose level</b>	125 mg/kg bw/d-no effects; 250 mg/kg bw/d-no effects; 500 mg/kg bw/d-body weight decrease compared to control
<b>Statistical evaluations</b>	Bartlett's test of homogeneity, ANOVA (F-test); alpha= 0.05
<b>Conclusion remarks</b>	The NOAEL for maternal toxicity was reported to be 125 mg/kg bw/d, and the NOAEL for offspring toxicity was 250 mg/kg bw/d.
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.

<b>Remarks for Data Reliability</b>	Acceptable, well documented publication, which meets basic scientific principles. Study duration shorter than guideline studies and less animals used.
<b>References</b>	Vollmuth T.A., Bennett, M.B., Hoberman, A.M. and Christian, M.S. (1995) An Evaluation of Food Flavoring Ingredients Using an In Vivo Reproductive and Developmental Toxicity Screening Test. Teratology 41(5): 597.

<b>Substance Name</b>	Citral
<b>CAS</b>	5392-40-5
<b>Remarks for Substance</b>	Substance supported under SIDS. 95% pure
<b>Test Type</b>	Embryo-feto toxicity
<b>GLP</b>	NG
<b>Year</b>	1995
<b>Species/Strain</b>	Wistar rats
<b>Sex</b>	Male and Female
<b>Route of administration</b>	Oral
<b>Duration of test</b>	21 days
<b>Doses/concentration levels</b>	0, 60, 125, 250, 500, and 1000 mg/kg bw in corn oil
<b>Exposure period</b>	Once a day for days 6-15 of pregnancy
<b>Frequency of treatment</b>	Daily
<b>Control Group and treatment</b>	Yes, the control group received only corn oil.
<b>Remarks for test conditions</b>	Citral was administered orally at the dose levels specified to female Wistar rats on days 6-15 of pregnancy. Caesarean sections were performed on day 21. Numbers of resorption and implantation sites were recorded. Fetuses were weighed and examined for gross malformations, visceral and skeletal malformations. Exposure to citral was limited to the main period of organogenesis.
<b>NOAEL(NOEL) maternal</b>	<60 mg/kg bw/d
<b>LOAEL(LOEL) maternal</b>	60 mg/kg bw/d
<b>NOAEL (NOEL) developmental</b>	<60 mg/kg bw/d
<b>LOAEL (LOEL) developmental</b>	60 mg/kg bw/d
<b>Actual dose received by dose level and sex</b>	NG
<b>Maternal data with dose level</b>	Statistically significant reductions in pregnancy weight gain (minus uterus weight) were reported for the two highest dose levels (500 and 1000 mg/kg bw/d) administered. Statistically significant differences in weight gain were reported for the other dose levels tested.

<b>Fetal data with dose level</b>	dose levels tested. Statistically significant reductions in fetal body weight were reported for dose levels at 125, 250, and 500 mg/kg bw/d. Increases in the frequency of delayed ossifications were reported for the 125 and 250 mg/kg bw/d and were statistically significant. The incidence of hematomas was significantly increased in animals receiving 250, 500 or 1000 mg/kg bw/d. The only fetal organ with treatment related reductions in weight were spleens at doses of 250 mg/kg bw/d or higher. Statistically significant increases in the number of fetuses showing skeletal abnormalities was reported for the 125, 250 and 1000 mg/kg bw/d dose levels. No treatment related effects were reported on the occurrence of gross structural abnormalities, or visceral malformations.
<b>Statistical evaluations</b>	One way ANOVA (F-test), or the Kruskal- Alpha value of 0.05.
<b>Remarks for results</b>	The authors hypothesized the later start day for treatment administration may have reduced in the induction of metabolic enzymes responsible for detoxification of citral.
<b>Conclusion remarks</b>	The NOAEL for developmental toxicity for citral is reported to be less than 60 mg/kg bw/d.
<b>Data Qualities Reliabilities</b>	Reliability code 2. Reliable with restrictions.
<b>Remarks for Data Reliability</b>	Acceptable, well documented publication, which meets basic scientific principles. Exposure to test material limited to main period of organogenesis.
<b>References</b>	Cristina A., Nogueira A.M., Carvalho R., Souza A., Chahoud I., Paumgarten F. (1995) Study on the embryofeto-toxicity of citral in the rat. Toxicology, 96, 105-113.

<b>Substance Name</b>	Citral
<b>CAS</b>	5392-40-5
<b>Remarks for Substance</b>	Substance supported under SIDS. Commercially available citral. Purity > 90%. Isomeric distribution of approximately 35% neral and 55% geranial.
<b>Method/guideline</b>	Not given
<b>GLP</b>	No
<b>Year</b>	1989
<b>Species/Strain</b>	Rat/Sprague-Dawley
<b>Sex</b>	Female
<b>Route of administration</b>	Inhalation
<b>Duration of test</b>	20 days
<b>Doses/concentration levels</b>	0, 10, 35 ppm as vapor or 85 ppm as aerosol/vapor

<b>Exposure period</b>	6 hr/day on gestational days 6-15
<b>Frequency of treatment</b>	Daily
<b>Control Group and treatment</b>	Yes
<b>Remarks for test conditions</b>	Pregnant Sprague Dawley rats were exposed via inhalation to 0, 10, 35, or 85 ppm citral for six hours a day on gestational days 6-15. Dams were sacrificed on day 20. Fetuses were examined for gross, visceral and skeletal malformations.
<b>NOAEL(NOEL) maternal</b>	35 ppm
<b>LOAEL(LOEL) maternal</b>	85 ppm
<b>NOAEL (NOEL) developmental toxicity</b>	85 ppm
<b>LOAEL (LOEL) developmental toxicity</b>	None reported
<b>Actual dose received by dose level and sex</b>	10.2 +/- 0.9 ppm, 34.4 +/- 4.1 ppm, 68 ppm (30.7 +/-4.2 ppm citral aerosol and 37.0 +/-14.1 ppm citral vapor)
<b>Maternal data with dose level</b>	At the 85 ppm dose level, a statistically significant ( $p<0.05$ ) difference in maternal weight gain for the dosed compared to the controls was reported. Additional signs of clinical toxicity were also reported. No toxicity was reported for the animals receiving 10 or 35 ppm citral.
<b>Fetal data with dose level</b>	No exposure related effects were reported on corpus lutea, implantations or resorptions, nor for fetal viability, litter size, sex ratio and body weight. No exposure related malformations were reported. The incidence of hypoplastic bones (lumbar and pubis) was increased slightly compared to the controls at the highest maternal dose level.
<b>Statistical evaluations</b>	Yes, ANOVA (F-test) and Fischers exact
<b>Remarks for results</b>	Citral administered via inhalation produced no teratogenic effects in rats at the dose levels tested.
<b>Conclusion remarks</b>	Citral administered via inhalation produced no teratogenic effects in rats at the dose levels tested.
<b>Data Qualities Reliabilities</b>	Reliability code 1. Reliable without restrictions.
<b>Remarks for Data Reliability</b>	Comparable to guideline study.
<b>References</b>	Gaworski C.L., Vollmuth, T.A., York R.G., Heck J.D., Arany C. (1992) Developmental toxicity evaluation of inhaled citral in rats. Food Chemical Toxicology, 30 269-275.